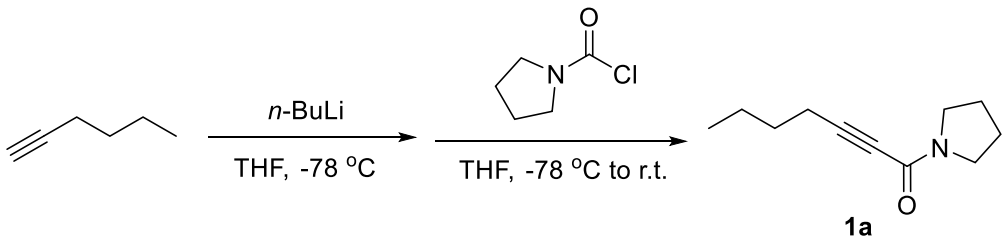
Content	Page number

General. Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous dichloromethane (HPLC grade), 1,2-dichloroethane (HPLC grade) were purified by distillation over calcium hydride. Toluene was distilled over sodium/benzophenone. Commercially available reagents were used without further purification. Reactions were monitored by thin-layer chromatography (TLC) using Silicycle precoated silica gel plates. Flash column chromatography was performed over Silicycle silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian 400 MHz, 500 MHz and 600 MHz spectrometers using residue solvent peaks as internal standards ($CHCl_3$, ^{1}H: 7.26 ppm; ^{13}C: 77.16 ppm). Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Xevo G2-XS QTOF Quadrupole Time-of-Flight Mass Spectrometry using electron spray ionization.

Preparation of substrates

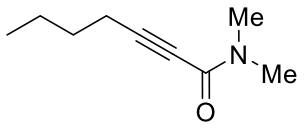
1-(Pyrrolidin-1-yl)hept-2-yn-1-one (1a)



To a stirred solution of 1-hexyne (6 mmol) and THF (15 mL) was added *n*-BuLi (2.4 mL, 6 mmol, 2.5 M in hexane) at -78 °C. After 20 min, the solution was slowly cannulated into pyrrolidine-1-carbonyl chloride (0.682g, 6 mmol)[1] in THF (15 mL) at -78°C. Then, the solution was allowed to warm up and stirred for 2 hours at rt. After that, the mixture was quenched with sat. aq. NH_4Cl (20 mL) and extracted with EtOAc (20 mL). The organic phase was dried (with $MgSO_4$), concentrated and purified by chromatography to give **1a** in 90% yield (0.97 g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.64 – 3.52 (m, 2H), 3.42 (t, *J* = 6.6 Hz, 2H), 2.31 (t, *J* = 7.0 Hz, 2H), 1.88 (dq, *J* = 6.4, 3.8, 2.8 Hz, 4H), 1.57 – 1.46 (m, 2H), 1.40 (ddd, *J* = 9.9, 7.7, 6.0 Hz, 2H), 0.88 (t,

J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.00, 91.59, 75.22, 48.15, 45.19, 29.95, 25.42, 24.79, 21.99, 18.55, 13.55. IR (neat): 2957, 2874, 1624, 1415, 1339, 1224, 831, 734. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{11}H_{18}NO]^+$,180.1383; found 180.1388.

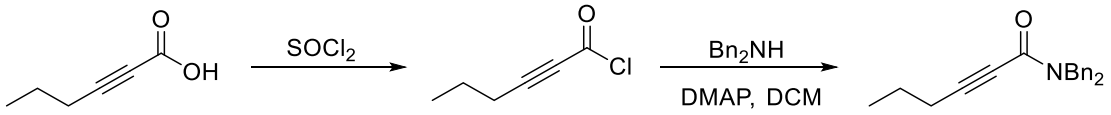
***N*,*N*-Dimethylhept-2-ynamide (1b)**



1b

Compound **1b** was prepared from 1-hexyne (5 mmol) and dimethylcarbamic chloride[1] (5 mmol) according to the preparative procedure for **1a** in 85% yield (0.65 g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.17 (s, 3H), 2.94 (s, 3H), 2.34 (t, *J* = 7.1 Hz, 2H), 1.61 – 1.50 (m, 2H), 1.47 – 1.35 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.92, 93.19, 74.13, 38.43, 34.11, 29.95, 22.09, 18.70, 13.60. IR (neat): 2961, 2935, 1643, 1396, 1269, 1189, 735. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_9H_{15}NONa]^+$, 176.1046; found 176.1058.

***N*,*N*-Dibenzylhept-2-ynamide (1c)**

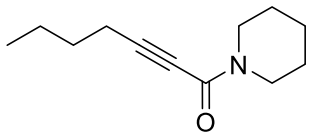


1c

A solution of 2-hexynoic acid (2.0 mmol) in $SOCl_2$ (2 mL) was stirred at 60 °C for 2 h. The mixture was cooled down to rt, and vapor away $SOCl_2$ to give the crude 2-hexynoic chloride, which was directly used in next step. To the solution of 2-hexynoic chloride in DCM (4 mL), dibenzylamine (3.0 mml, 1.5 equiv.) was slowly added at 0°C. Then, the solution was allowed to warm up and stirred at rt for 2 hours. After that, the mixture was quenched with sat. aq. NH_4Cl (10 mL), diluted with EtOAc (10 mL). The organic phase was dried (with $MgSO_4$), concentrated and purified by chromatography to give **1c** (220 mg, 39% yield for 2 steps). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.14 (m, 5H), 4.67 (s, 1H), 4.50 (s, 1H), 2.34 (t, *J* = 7.0 Hz, 1H), 1.58 (q, *J* = 7.2 Hz, 1H),

0.96 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.31, 136.54, 136.39, 128.94, 128.78, 128.58, 127.99, 127.81, 127.70, 93.90, 74.34, 51.45, 46.29, 21.44, 21.11, 13.67. IR (neat): 3009, 2182, 1622, 1493, 1419, 1235, 693. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{20}H_{22}NO]^+$, 292.1696; found 292.1704.

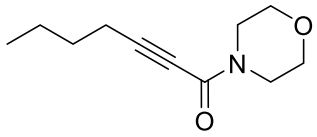
1-(Piperidin-1-yl)hept-2-yn-1-one (1d)



1d

Compound **1d** was prepared from 1-hexyne (5 mmol) and piperidine-1-carbonyl chloride[1] (5 mmol) according to the procedure for **1a** in 47% yield (0.45 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 3.71 – 3.64 (m, 2H), 3.60 – 3.52 (m, 2H), 2.36 (t, *J* = 7.1 Hz, 2H), 1.70 – 1.51 (m, 9H), 1.48 – 1.37 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.20, 93.21, 73.91, 48.16, 42.26, 29.95, 26.46, 25.44, 24.63, 22.09, 18.75, 13.60. IR (neat): 2939, 2859, 1635, 1466, 1368, 1235, 853, 732. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{12}H_{19}NONa]^+$, 216.1359; found 216.1374.

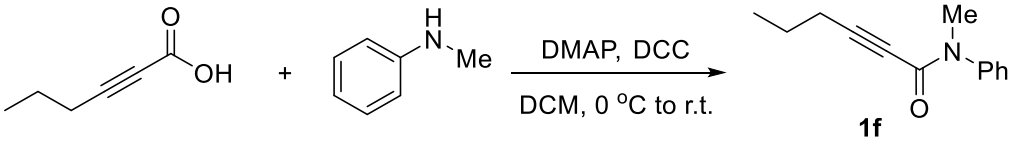
1-Morpholinohept-2-yn-1-one (1e)



1e

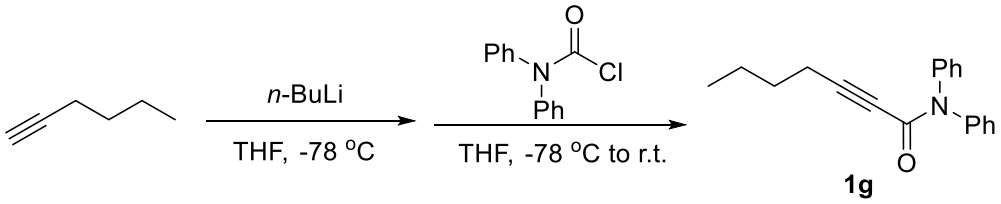
Compound **1e** was prepared from 1-hexyne (5 mmol) and morpholine-4-carbonyl chloride[1] (5 mmol) according to the procedure for **1a** in 52% yield (0.50 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 3.85 – 3.50 (m, 8H), 2.36 (t, *J* = 7.1 Hz, 2H), 1.56 (q, *J* = 7.0 Hz, 2H), 1.49 – 1.36 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.36, 94.23, 73.29, 66.89, 66.49, 47.23, 41.83, 29.82, 22.05, 18.66, 13.53. IR (neat): 2960, 2860, 1635, 1428, 1247, 830, 731. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{11}H_{18}NO_2]^+$, 196.1332; found 196.1336.

***N*-Methyl-*N*-phenylhex-2-ynamide (1f)**



To a solution of 2-hexynoic acid (7.5 mmol, 1 equiv.) and *N*-methyl aniline (8.0 mmol) in 3 mL of DCM (10 mL) at 0 °C, DCC (1.1 equiv.) and DMAP (0.1 equiv.) were added slowly. The reaction mixture was warmed up and stirred at r.t. for 12 h. After that, the mixture was filtrated, washed with DCM. The filtrate was evaporated and the residue was purified by flash column chromatography to give corresponding ynamide **1f** (1.04 g, 69% yield). For the major rotamer, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.36 (m, 2H), 7.35 – 7.24 (m, 3H), 3.32 (s, 3H), 2.07 (t, *J* = 6.9 Hz, 2H), 1.28 (h, *J* = 7.2 Hz, 2H), 0.70 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.52, 143.49, 129.14, 127.77, 127.36, 93.98, 75.11, 36.41, 21.01, 20.79, 13.22. IR (neat): 3067, 2966, 1643, 1596, 1495, 1369, 1175, 1095, 770. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_9H_{15}NONa]^+$, 176.1046; found 176.1058.

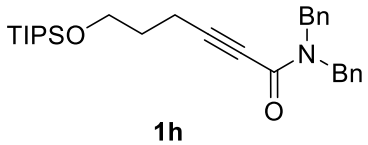
***N*,*N*-Diphenylhept-2-ynamide (1g)**



To a stirred solution of 1-hexyne (4 mmol) and THF (10 mL) was added *n*-BuLi (1.6 mL, 4.00 mmol, 2.5 M in hexane) at -78 °C. After 20 min, the solution was slowly cannulated into $ClC(O)NPh_2$ (924 mg, 4 mmol)[1] in THF (10 mL) at -78°C. Then, the solution was allowed to warm up and stirred for 2 hours at rt. After that, the mixture was quenched with sat. aq. NH_4Cl (20 mL), diluted with EtOAc (20 mL). The organic phase was dried (with $MgSO_4$), concentrated and purified by chromatography to give **1g** (460 mg, 42% yield). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.32 – 7.19 (m, 10H), 2.14 (t, *J* = 6.9 Hz, 2H), 1.24 (dqd, *J* = 8.6, 6.8, 0.6 Hz, 2H), 1.14 – 1.02 (m, 2H), 0.77 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.91, 142.61, 141.47, 129.09,

129.02, 127.93, 126.42, 126.02, 95.74, 75.72, 29.43, 21.61, 18.64, 13.55. IR (neat): 2958, 2932, 1648, 1491, 1340, 1029, 757. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{20}H_{22}NO]^+$, 292.1696; found 292.1704.

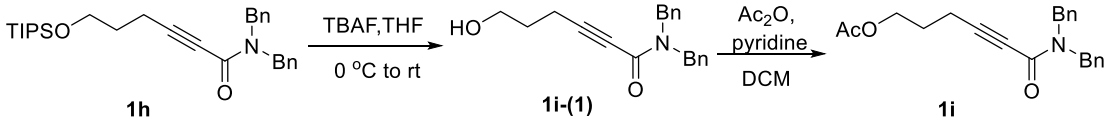
N,N-Dibenzyl-6-((triisopropylsilyl)oxy)hex-2-ynamide (1h)



1h

Compound **1h** was prepared from triisopropyl(pent-4-yn-1-yloxy)silane (5.77 mmol) and dibenzylcarbamic chloride (5.77 mmol) according to the procedure for **1b** in 86% yield (2.36 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43 – 7.06 (m, 10H), 4.67 (s, 2H), 4.50 (s, 2H), 3.72 (t, *J* = 5.9 Hz, 2H), 2.50 (t, *J* = 7.1 Hz, 2H), 1.84 – 1.73 (m, 2H), 1.14 – 0.96 (m, 21H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.21, 136.49, 136.32, 128.91, 128.74, 128.52, 127.96, 127.75, 127.66, 93.80, 74.16, 61.68, 51.43, 46.23, 31.19, 18.08, 15.65, 12.02. IR (neat): 2943, 2892, 2866, 1635, 1421, 1233, 1073, 882, 732. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{29}H_{42}NO_2Si]^+$, 464.2979; found 464.2984..

6-(Dibenzylamino)-6-oxohex-4-yn-1-yl acetate (1i)

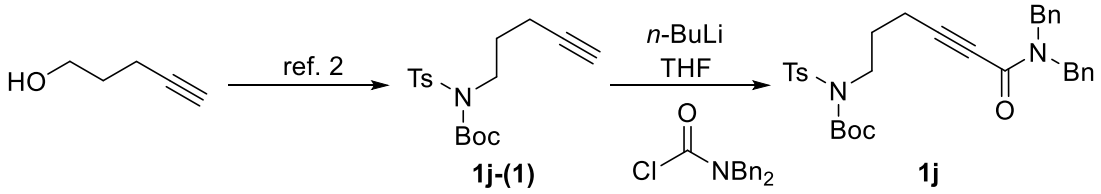


1h **1i-(1)** **1i**

Compound **1i** was prepared from **1h**. To the solution of **1h** (1.5 g, 3.23 mmol) in THF (20 mL) was added TBAF (1.1 equiv.) at 0 °C and then stirred at rt for 1h. After that, water (20 mL) was added and extracted with ethyl acetate (20 mL). The organic phase was washed with brine and dried with $MgSO_4$ before concentrating. The crude product was purified by chromatography to give the alcohol **1i-(1)** (0.92 g, 93%). To the solution of the alcohol **1i-(1)** (0.6 mmol) in DCM (10 mL) was added Ac_2O (0.72 mmol), then pyridine (1.5 equiv.) and DMAP (0.1 equiv.). The mixture was stirred at r.t. for 2h before adding brine (10 mL). The organic phase was dried with $MgSO_4$ and condensed. Further purification by chromatography gave the product **1i**

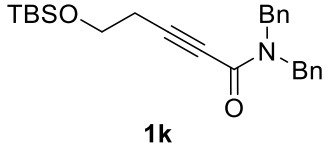
(199 mg, 95%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.15 (m, 10H), 4.66 (s, 2H), 4.50 (s, 2H), 4.09 (t, *J* = 6.2 Hz, 2H), 2.46 (t, *J* = 7.1 Hz, 2H), 2.01 (s, 3H), 1.93 – 1.78 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.80, 154.84, 136.23, 136.08, 128.80, 128.62, 128.39, 127.86, 127.57, 127.51, 92.01, 74.57, 62.70, 51.28, 46.25, 26.91, 20.80, 15.86.IR (neat): 2928, 2239, 1736, 1623, 1420, 1230, 698. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{22}H_{24}NO_3]^+$, 350.1751; found 350.1747.

***tert*-Butyl (6-(dibenzylamino)-6-oxohex-4-yn-1-yl)(tosyl)carbamate (1j)**



Compound **1j** was prepared from **1j-(1)**[2] (1 mmol) and dibenzylcarbamic chloride[1] (1 mmol) according to the procedure for **1b** in 56% yield (309 mg). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 – 7.67 (m, 2H), 7.44 – 7.21 (m, 12H), 4.76 (s, 2H), 4.54 (s, 2H), 3.98 – 3.82 (m, 2H), 2.51 (t, *J* = 7.2 Hz, 2H), 2.45 (s, 3H), 2.14 – 1.99 (m, 2H), 1.34 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.91, 150.74, 144.22, 137.11, 136.29, 136.23, 129.26, 128.78, 128.62, 128.37, 127.79, 127.72, 127.68, 127.54, 92.13, 84.40, 74.58, 51.35, 46.20, 46.13, 28.29, 27.82, 21.58, 16.60. IR (neat): 2981, 2933, 1727, 1628, 1495, 1286, 988, 814, 735. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{32}H_{36}N_2O_5SNa]^+$, 583.2237; found 583.2226.

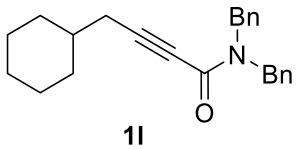
***N*, *N*-Dibenzyl-5-((tert-butyldimethylsilyl)oxy)pent-2-ynamide (1k)**



Compound **1k** was prepared from (but-3-yn-1-yloxy)(tert-butyl)dimethylsilane (3 mmol) and dibenzylcarbamic chloride[1] (3 mmol) according to the procedure for **1b** in 60% yield (0.55 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.40 – 7.19 (m, 10H), 4.69 (s, 2H), 4.51 (s, 2H), 3.77 (t, *J* = 6.9 Hz, 2H), 2.59 (t, *J* = 6.8 Hz, 2H), 0.86 (s, 9H), 0.04

(s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.03, 136.41, 136.25, 128.90, 128.75, 128.49, 127.97, 127.82, 127.67, 90.99, 74.98, 60.96, 51.44, 46.20, 25.91, 23.56, 18.33, -5.29. IR (neat): 2954, 2929, 2856, 1633, 1423, 1251, 1075, 837, 753. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{25}H_{34}NO_2S]^+$, 408.2353; found 408.2357.

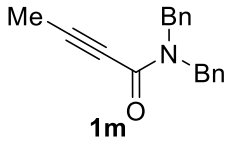
***N*, *N*-Dibenzyl-4-cyclohexylbut-2-ynamide (1l)**



1l

Compound **1l** was prepared from prop-2-yn-1-ylcyclohexane (3 mmol) and dibenzylcarbamic chloride[1] (3 mmol) according to the procedure for **1b** in 63% yield (1.0 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43 – 7.21 (m, 10H), 4.70 (s, 2H), 4.53 (s, 2H), 2.27 (d, J = 6.6 Hz, 2H), 1.80 – 1.46 (m, 6H), 1.27 – 0.91 (m, 5H). ^{13}C NMR (126 MHz, Chloroform-d) δ 155.33, 136.54, 136.36, 128.86, 128.72, 128.54, 127.88, 127.64, 127.62, 92.98, 75.07, 51.37, 46.37, 36.89, 32.75, 26.83, 26.07, 26.05. IR (neat): 2923, 2851, 2238, 1712, 1624, 1420, 1213, 729, 697. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{24}H_{27}NNaO]^+$,368.1985; found 368.1951.

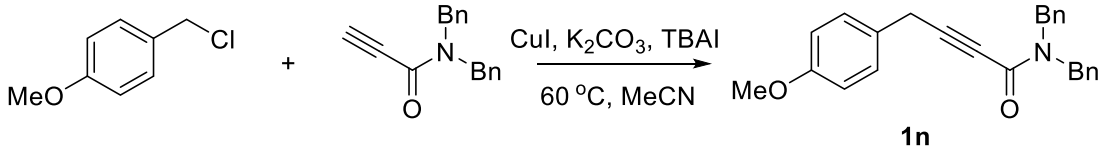
***N*, *N*-Dibenzylbut-2-ynamide (1m)**



1m

Crude 2-butynoic chloride was prepared from 2-butynoic acid (2.0 mmol) in $SOCl_2$ (2 mL) and directly used with dibenzylamine (3.0 mmol, 1.5 equiv.) according to the procedure for **1c** in 50% yield (0.26 g). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.45 – 7.16 (m, 10H), 4.68 (s, 2H), 4.51 (s, 2H), 2.02 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 155.20, 136.42, 136.30, 128.92, 128.75, 128.49, 127.98, 127.76, 127.67, 89.86, 73.48, 51.37, 46.20, 4.23.δ IR (neat): 2922, 2242, 1615, 1419, 1225, 973, 732, 696. MS-ESI (m/z): $[M+Na]^+$ calcd. for $[C_{18}H_{17}NNaO]$+,286.1202; found 286.1195.

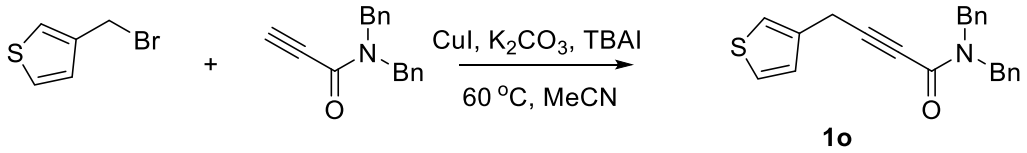
N,N-dibenzyl-4-(4-methoxyphenyl)but-2-ynamide (1n)



1n

To a dried, Ar protected Schlenk flask were added sequentially CuI (190 mg, 1 mmol), K_2CO_3 (138 mg, 1 mmol), TBAI (370 mg, 1 mmol). N,N-dibenzylpropiolamide (500 mg, 2 mmol) was dissolved in 5 mL degassed MeCN and injected. 1-(chloromethyl)-4-methoxybenzene (156.61 mg, 1 mmol) was injected last. The reaction was heated at 60 °C for 24 hrs, then washed with saturated NH_4Cl solution. 280 mg **1n** was obtained with 76% Yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.42 – 7.20 (m, 10H), 7.19 – 7.11 (m, 2H), 6.84 – 6.68 (m, 2H), 4.68 (s, 2H), 4.54 (s, 2H), 3.77 (s, 3H), 3.71 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.69, 155.07, 136.38, 136.22, 129.01, 128.90, 128.83, 128.74, 128.58, 128.52, 127.94, 127.69, 127.65, 127.36, 126.62, 114.19, 91.40, 75.69, 55.36, 51.39, 46.44, 24.61. IR (neat): 2836, 2239, 1624, 1450, 1421, 1245, 698. MS-ESI (m/z): $[M+Na]^+$ calcd. for $[C_{25}H_{23}NNaO_2]^+$,392.1621; found 392.1624.

N,N-dibenzyl-4-(thiophen-3-yl)but-2-ynamide (1o)

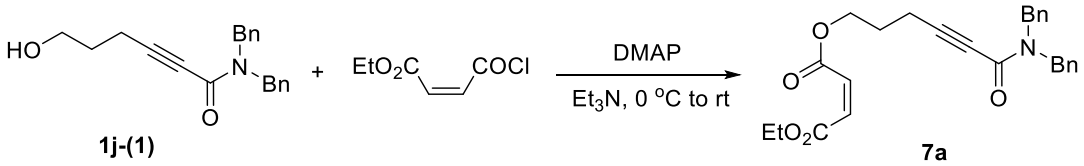


1o

To a dried, Ar protected Schlenk flask were added sequentially CuI (190 mg, 1 mmol), K_2CO_3 (138 mg, 1 mmol), TBAI (370 mg, 1 mmol). N,N-dibenzylpropiolamide (250mg, 1 mmol) was dissolved in 5 mL degassed MeCN and injected. 3-(bromomethyl)thiophene (212.5 mg, 1 mmol) was injected last. The reaction was heated at 60 °C for 24 hr, then washed with saturated NH_4Cl solution. 100 mg **1o** was obtained with 29% yield and 89% purity along with some inseparable unknown impurities. ^{1}H NMR (600 MHz, Chloroform-d) δ 7.43 – 7.14 (m, 11H), 7.05 (dq, J = 2.5, 1.2 Hz, 1H), 6.94 (dd, J = 5.0, 1.3 Hz, 1H), 4.69 (s, 2H), 4.54 (s, 2H), 3.75 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.88, 136.23, 136.07, 134.38, 128.86, 128.67, 128.43, 127.89,

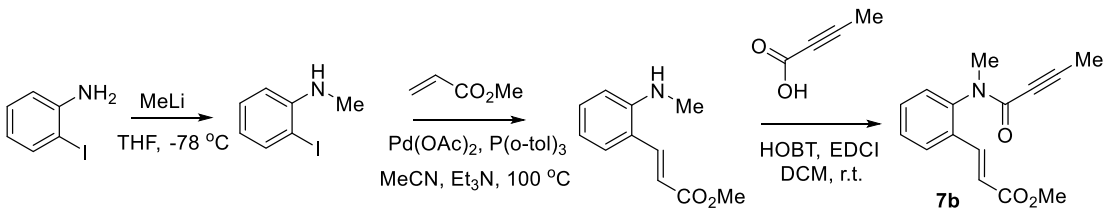
127.63, 127.51, 127.36, 126.28, 90.49, 75.24, 51.28, 46.38, 20.49. IR: 3029, 2924, 2240, 1710, 1622, 1420, 1232, 697. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{22}H_{19}NNaOS]^+$, 368.1080; found 368.1084.

6-(Dibenzylamino)-6-oxohex-4-yn-1-yl ethyl maleate (7a)



Ethyl (*Z*)-4-chloro-4-oxobut-2-enoate **7a** was prepared according to the procedure for (*E*)-4-chloro-4-oxobut-2-enoate.[3] At 0 °C, to the solution of **1j-(1)** (0.7 mmol) in DCM (10 mL) was added ethyl (Z)-4-chloro-4-oxobut-2-enoate (0.7 mmol), then Et_3N (1.5 equiv.) and DMAP (0.1 equiv.) were added. The mixture was stirred at r.t. for 2 h before adding brine (10 mL). The organic phase was dried with $MgSO_4$ and condensed. Further purification by chromatograph gave the product **7a** (166 mg, 55%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43 – 7.14 (m, 10H), 6.81 (s, 2H), 4.66 (s, 2H), 4.50 (s, 2H), 4.34 – 4.19 (m, 4H), 2.49 (t, *J* = 7.1 Hz, 2H), 2.00 – 1.89 (m, 2H), 1.31 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.88, 164.80, 154.89, 136.32, 136.15, 134.12, 133.11, 128.93, 128.75, 128.51, 127.98, 127.70, 127.58, 91.70, 74.88, 63.59, 61.47, 51.40, 46.41, 26.91, 15.88, 14.19. IR (neat): 2982, 2938, 1721, 1631, 1496, 1423, 1260, 1030, 978, 733. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{26}H_{28}NO_5]^+$, 434.1962; found 434.1948.

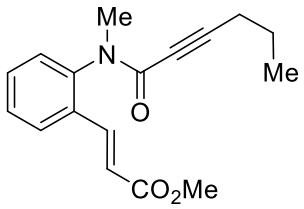
Methyl (E)-3-(2-(N-methylbut-2-ynamido)phenyl)acrylate (7b)



N-methyl-2-iodoaniline was prepared according to the procedure previously reported.[4] A mixture of N-methyl-2-iodoaniline (3.0g, 12.87 mmol) methylacrylate (1.33g,

15.44mmol), $Pd(OAc)_2$ (143.7 mg, 0.64 mmol), Et_3N (2.135 ml, 15.44 mmol), and P(o-tol)$_3$ (292mg, 0.96 mmol) in anhydrous CH_3CN (20 ml) was heated for 6 hrs in a tightly capped culture tube under Ar atmosphere. The mixture was portioned between Et_2O and a 1:1 mixture of 3 N HCl and brine. The crude product was purified by flash column chromatography gave methyl (E)-3-(2-(dimethylamino) phenyl) acrylate (1.87g, 71%). 2-butynoic acid (168 mg, 2.0 mmol), EDCI (1.2 eq) and HOBT (0.1 eq) were added to a solution of methyl (E)-3-(2-(dimethylamino) phenyl) acrylate (1.0 eq) in DCM (0.25 M) at room temperature, The resulting solution was stirred at room temperature for 20 hours, quenched with $NaHCO_3$ ($_{aq.}$) and extracted twice with DCM. The combined organic layers were washed with water and brine, dried over Na_2SO_4, concentrated in vacuo and purified by flash chromatography on silica gel to afford **7b** in 62% yield (320 mg). ^{1}H NMR (500 MHz, Chloroform-d)(Major rotamer) δ 7.70 – 7.56 (m, 2H), 7.47 – 7.31 (m, 2H), 7.27 – 7.16 (m, 1H), 6.43 (d, J = 16.0, 1H), 3.79 (s, 3H), 3.23 (s, 3H), 1.65 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 166.86, 154.69, 142.53, 139.11, 132.81, 131.12, 129.53, 128.98, 127.46, 120.92, 90.54, 73.98, 51.99, 36.54, 3.93. IR (neat): 2998, 2225, 1702, 1624, 1364, 1270, 981, 775, 735, 594. $[M+Na]^+$ calcd. for $[C_{15}H_{15}NNaO_3]^+$, 280.0944; found 280.0953.

Methyl (E)-3-(2-(N-methylhex-2-ynamido)phenyl)acrylate (7c)

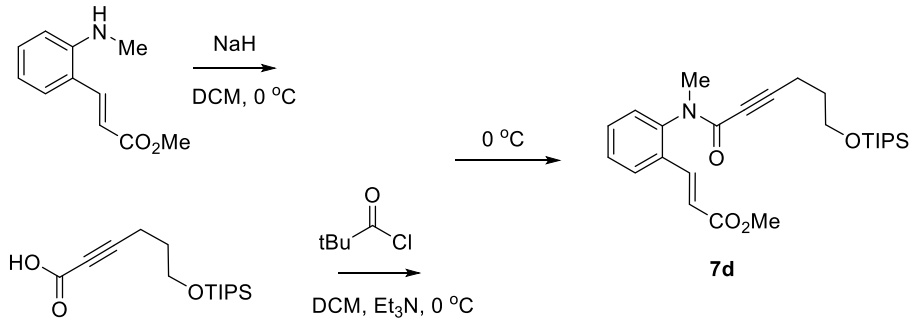


7c

Compound **7c** was prepared according to the procedure 7b by using 2-hexynoic acid (224 mg, 2 mmol) in the last step. Compound **7c** was afforded in 65% yield (372 mg). ^{1}H NMR (500 MHz, Chloroform-d)) (Major rotamer) δ 7.71 – 7.56 (m, 2H), 7.46 – 7.31 (m, 2H), 7.27 – 7.15 (m, 1H), 6.42 (d, J = 16.0 Hz, 1H), 3.78 (s, 3H), 3.24 (s, 3H), 1.98 (t, J = 6.9 Hz, 2H), 1.16 (h, J = 7.2 Hz, 2H), 0.60 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 166.81, 154.72, 142.67, 139.08, 132.90, 131.10, 129.55,

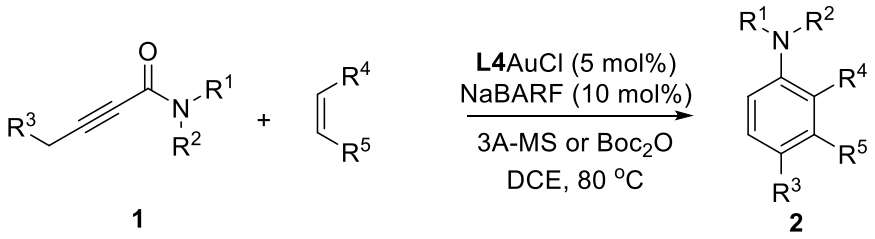
128.93, 127.37, 120.89, 94.55, 74.93, 51.95, 51.95, 36.42, 20.96, 20.68, 13.11. IR (neat): 2964, 2223, 1716, 1634, 1272, 1171, 1036, 763, 733, 589. $[M+Na]^+$ calcd. for $[C_{17}H_{19}NNaO_3]^+$, 308.1257; found 308.1255.

Methyl (E)-3-(2-(N-methyl-6-((triisopropylsilyl)oxy)hex-2ynamido)phenyl) acrylate (7d)



1.0 equiv. N-methyl-2-iodoaniline methylacrylate (235mg, 1.23 mmol) was dissolved in 6 ml DCM under Ar atmosphere, NaH 60% in oil (73.8mg, 1.84 mmol) was added at 0 °C, keep stirring at room temperature for another 45 minutes. 2.0 equiv. 6-((triisopropylsilyl)oxy) hex-2-ynoic acid (700 mg, 2.46 mmol) was dissolved in 6 ml DCM under Ar, Et_3N (273 mg, 2.70 mmol) was added, then pivaloyl chloride (326 mg, 2.70 mmol) was added. Keep stirring for 20 minutes. Then deprotonated N-methyl-2-iodoaniline methylacrylate was transferred to the reaction via cannula at 0 °C. The reaction was stirred overnight. **7d** (350 mg, 62%) was obtained by flash chromatography. ^{1}H NMR (500 MHz, Chloroform-d) (Major rotamer) δ 7.72 – 7.57 (m, 2H), 7.48 – 7.35 (m, 2H), 7.26 (m, 1H), 6.44 (d, J = 16.0, 1H), 3.80 (s, 3H), 3.39 (t, J = 5.8 Hz, 2H), 3.25 (s, 3H), 2.15 (t, J = 7.0 Hz, 2H), 1.40 – 1.29 (m, 2H), 1.11 – 1.04 (m, 3H), 0.99 (d, J = 3.2 Hz, 18H). ^{13}C NMR (126 MHz, Chloroform-d) δ 166.75, 154.63, 142.67, 139.01, 132.84, 131.03, 129.59, 128.92, 127.32, 120.89, 94.58, 74.68, 61.26, 51.94, 36.42, 31.00, 18.10, 18.03, 18.02, 15.17, 11.96. IR (neat): 2943, 2865, 2225, 1719, 1640, 1171, 1104, 882, 733, 680. . $[M+Na]^+$ calcd. for $[C_{26}H_{39}NNaO_4Si]^+$, 480.2541; found 480.2537.

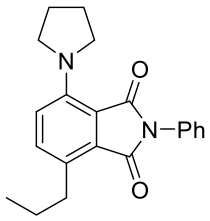
Gold-catalyzed intermolecular ynamide isomerization and D-A reactions with dienophiles



1 2

General procedure A: To a dried, Ar protected Schlenk tube were added sequentially 0.15 mmol ynamide **1**, 0.30 mmol dienophile (2 equiv.), 0.0075-0.0150 mmol **L4**AuCl (5-10 mol%), 0.015-0.030 mmol NaBARF (10-20 mol%), 3Å molecular sieves or Boc_2O and 3 mL anhydrous DCE. The reaction was then heated at the 80 °C for 12-24 h and monitored by TLC or NMR. The reaction was concentrated under reduced pressure. The residue was purified through silica gel flash chromatography to obtain the pure product **2** or **6**.

2-Phenyl-4-propyl-7-(pyrrolidin-1-yl)isoindoline-1,3-dione (2a)

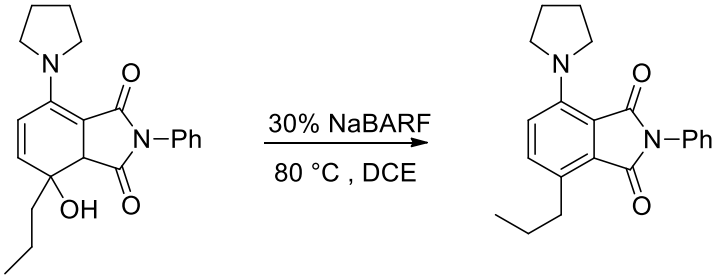


2a

Compound **2a** was prepared following general procedure A. The reaction was heated at 80 °C for 18 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2a** (36.6 mg) in 73% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.52 – 7.45 (m, 2H), 7.45 – 7.40 (m, 2H), 7.38 – 7.33 (m, 1H), 7.30 (d, *J* = 8.8 Hz, 1H), 6.96 (d, *J* = 8.7 Hz, 1H), 3.64 – 3.54 (m, 4H), 3.07 – 2.96 (m, 2H), 2.03 – 1.94 (m, 4H), 1.72 – 1.61 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.04, 166.93, 145.52, 137.14, 132.49, 131.86, 129.72, 128.97, 127.66, 127.13, 120.91, 111.45, 51.91, 32.75, 25.93, 24.33, 14.14. IR (neat): 2960, 2929, 2869, 1702, 1642, 1501, 1375, 1190,

1115, 939, 765. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{21}H_{23}N_2O_2]^+$, 335.1754; found 335.1741.

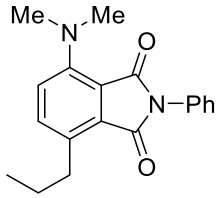
4-Hydroxy-2-phenyl-4-propyl-7-(pyrrolidin-1-yl)-3a,4-dihydro-1H-isoindole-1,3(2H)-dione (2a')



2a' **2a**

The labile **2a'** was separated from compound **2a** by column chromatography. ^{1}H NMR (600 MHz, Chloroform-d) δ 7.48 – 7.43 (m, 2H), 7.37 – 7.31f (m, 3H), 6.39 (d, J = 10.1 Hz, 1H), 6.18 (d, J = 10.1 Hz, 1H), 4.61 – 3.32 (bs, 2H, a 1H singlet at 3.90 and a 2H multiplet at 3.62 – 3.51), 3.04 (s, 1H, OH), 2.16 – 2.00 (m, 2H), 1.84 (m, 3H), 1.65 – 1.54 (m, 1H), 1.41 (ddd, J = 13.3, 12.2, 4.3 Hz, 1H), 1.31 – 1.23 (m, 1H), 0.87 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 175.71, 165.25, 148.20, 147.45, 133.04, 128.98, 128.97, 127.93, 127.66, 127.13, 127.01, 121.16, 120.89, 83.92, 74.66, 53.66, 51.90, 36.49, 32.74, 25.93, 25.63, 16.57, 14.73. IR (neat): 3440 (broad peak), 2957, 2870, 1666, 1533, 1338, 1094, 743, 614. MS-ESI (m/z): $[M+Na]^+$ calcd. for $[C_{21}H_{24}N_2NaO_3]^+$, 375.1679; found 375.1679. Compound **2a'** was converted to Compound **2a** under treatment of 30% NaBARF at 80 °C in DCE overnight confirmed by crude NMR.

4-(Dimethylamino)-2-phenyl-7-propylisoindoline-1,3-dione (2b)

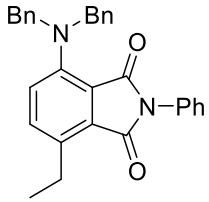


2b

Compound **2b** was prepared following general procedure A. The reaction was heated at 80 °C for 18 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.)

to give **2b** (39.7 mg) in 86% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.32 (m, 6H), 7.11 (d, *J* = 8.6 Hz, 1H), 3.07 (s, 6H), 3.05 – 2.98 (m, 2H), 1.67 (h, *J* = 7.4 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.92, 166.57, 149.40, 137.36, 133.98, 132.16, 129.73, 129.00, 127.76, 126.95, 122.65, 115.76, 43.75, 32.80, 24.27, 14.11. IR (neat): 3066, 1710, 1386, 1363, 1117, 760, 685, 626. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{19}H_{21}N_2O_2]^+$, 309.1598; found 309.1616.

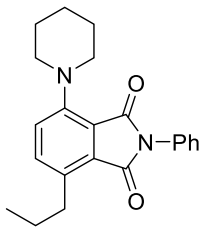
4-(Dibenzylamino)-7-ethyl-2-phenylisoindoline-1,3-dione (2c)



2c

Compound **2c** was prepared following general procedure A. The reaction was heated at 80 °C for 18 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc$_2$O (2 equiv.) to give **2c** (59.5 mg) in 89% yield.^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.56 – 7.46 (m, 6H), 7.43 – 7.20 (m, 18H), 7.16 (d, *J* = 8.8 Hz, 2H), 4.57 (s, 6H), 3.11 (q, *J* = 7.5 Hz, 3H), 1.29 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 167.83, 166.60, 148.11, 137.90, 136.66, 136.42, 132.17, 129.70, 129.05, 128.56, 128.17, 127.87, 127.32, 127.07, 126.15, 118.21, 56.61, 24.11, 14.99. IR (neat): 3028, 2931, 2967, 1705, 1642, 1496, 1381, 1191, 738. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{30}H_{27}N_2O_2]^+$, 447.2067; found 447.2083.

2-Phenyl-4-(piperidin-1-yl)-7-propylisoindoline-1,3-dione (2d)

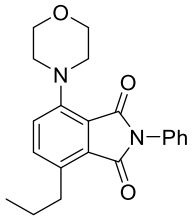


2d

Compound **2d** was prepared following general procedure A. The reaction was heated at 80 °C for 18 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc$_2$O (2 equiv.)

to give **2d** (42.8 mg) in 82% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.33 (m, 6H), 7.15 (d, *J* = 8.6 Hz, 1H), 3.24 (t, *J* = 5.3 Hz, 4H), 3.03 (dd, *J* = 8.6, 6.8 Hz, 2H), 1.80 (p, *J* = 5.6 Hz, 4H), 1.73 – 1.61 (m, 4H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.99, 166.71, 150.05, 137.57, 135.08, 132.12, 129.70, 129.08, 127.89, 127.09, 123.79, 118.22, 53.10, 32.89, 28.61, 26.18, 24.28, 24.18, 14.11. IR (neat): 2957, 2935, 2857, 1708, 1636, 1500, 1383, 1188, 931, 745. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{22}H_{25}N_2O_2]^+$, 349.1911; found 349.1915.

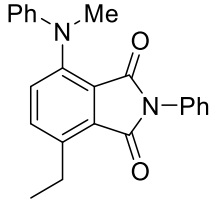
4-Morpholino-2-phenyl-7-propylisoindoline-1,3-dione (2e)



2e

Compound **2e** was prepared following general procedure A. The reaction was heated at 80 °C for 18 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc$_2$O (2 equiv.) to give **2e** (42.0 mg) in 80% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.31 (m, 6H), 7.15 (d, *J* = 8.5 Hz, 1H), 3.98 – 3.86 (m, 4H), 3.36 – 3.25 (m, 4H), 3.09 – 3.00 (m, 2H), 1.76 – 1.61 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.81, 166.78, 148.96, 137.89, 136.17, 131.94, 129.85, 129.18, 128.11, 127.07, 123.25, 118.80, 67.14, 51.82, 32.92, 24.28, 14.11. IR (neat): 2960, 2864, 1707, 1619, 1499, 1382, 1116, 935, 747. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{21}H_{22}N_2O_3Na]^+$, 373.1523; found 373.1542.

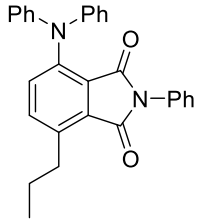
4-Ethyl-7-(methyl(phenyl)amino)-2-phenylisoindoline-1,3-dione (2f)



2f

Compound **2f** was prepared following general procedure A. The reaction was heated at 80 °C for 12 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and 3Å molecular sieves to give **2f** (50.2 mg) in 94% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.32 (m, 7H), 7.30 – 7.21 (m, 2H), 6.98 – 6.94 (m, 3H), 6.93 – 6.89 (m, 3H), 3.45 (s, 2H), 3.17 (q, *J* = 7.5 Hz, 3H), 1.33 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.55, 165.44, 148.12, 145.35, 140.46, 136.46, 132.58, 131.93, 129.60, 129.21, 129.05, 127.94, 126.87, 122.88, 120.58, 117.35, 41.05, 24.39, 15.08. IR (neat): 2966, 2931, 1708, 1643, 1493, 1379, 1188, 893,746. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{23}H_{20}N_2O_2Na]^+$, 379.1417; found 379.1418.

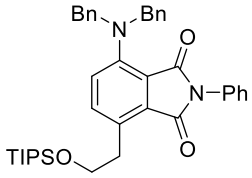
4-(Diphenylamino)-2-phenyl-7-propylisoindoline-1,3-dione (2g)



2g

Compound **2g** was prepared following general procedure A. The reaction was heated at 80 °C for 12 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and 3Å molecular sieves to give **2g** (62.9 mg) in 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.37 (m, 3H), 7.35 – 7.22 (m, 8H), 7.13 – 7.01 (m, 6H), 3.19 – 3.02 (m, 2H), 1.83 – 1.67 (m, 2H), 1.05 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.47, 164.28, 147.85, 143.37, 139.09, 137.40, 133.52, 131.86, 129.88, 129.31, 128.92, 127.73, 126.78, 123.65, 123.47, 123.45, 33.19, 24.23, 14.21. IR (neat): 3035, 2931, 1765, 1715, 1588, 1487, 1376, 1296, 1193, 1114, 753. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{29}H_{25}N_2O_2]^+$, 433.1880; found 433.1881.

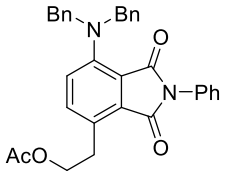
4-(Dibenzylamino)-2-phenyl-7-(2-((triisopropylsilyl)oxy)ethyl)isoindoline-1,3-dione (2h)



2h

Compound **2h** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2h** (65.8 mg) in 71% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.53 – 7.45 (m, 4H), 7.43 – 7.36 (m, 2H), 7.32 – 7.21 (m, 11H), 7.11 (d, *J* = 8.6 Hz, 1H), 4.56 (s, 4H), 3.99 (t, *J* = 6.0 Hz, 2H), 3.30 (t, *J* = 6.0 Hz, 2H), 0.98 (d, *J* = 6.1 Hz, 21H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.91, 166.64, 148.51, 138.88, 137.90, 132.25, 132.19, 130.28, 129.09, 128.58, 128.18, 127.91, 127.34, 127.09, 125.46, 117.99, 63.54, 56.69, 34.42, 18.10, 12.04. IR (neat): 2941, 2891, 2865, 1711, 1639, 1497, 1380, 1114, 884, 736. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{39}H_{46}N_2O_3SiNa]^+$, 641.3170; found 641.3182.

2-(7-(Dibenzylamino)-1,3-dioxo-2-phenylisoindolin-4-yl)ethyl acetate (2i)

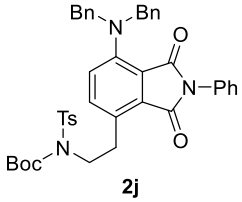


2i

Compound **2i** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (10 mol%), NaBARF (20 mol%) and Boc_2O (2 equiv.) to give **2i** (58.3 mg) in 77% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 – 7.44 (m, 4H), 7.42 – 7.37 (m, 1H), 7.35 – 7.21 (m, 11H), 7.13 (d, *J* = 8.6 Hz, 1H), 4.59 (s, 4H), 4.36 (t, *J* = 6.8 Hz, 2H), 3.40 (t, *J* = 6.8 Hz, 2H), 2.01 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.00, 167.71, 166.45, 148.76, 137.68, 137.61, 131.99, 130.68, 129.62, 129.08, 128.60, 128.12, 127.99, 127.39, 127.01, 125.82, 118.05, 64.10, 56.59, 30.24, 21.05. IR (neat): 2954, 2928, 2851, 1737, 1709, 1621, 1498, 1383, 1191, 1119,

1036, 887, 738. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{32}H_{29}N_2O_4]^+$, 505.2122; found 505.2131.

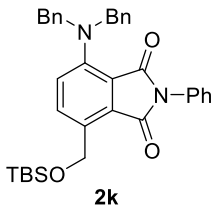
tert-Butyl-(2-(7-(dibenzylamino)-1,3-dioxo-2-phenylisoindolin-4-yl)ethyl)(tosyl)carbamate (2j)



2j

Compound **2j** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (10 mol%), NaBARF (20 mol%) and Boc_2O (2 equiv.) to give **2j** (81.5 mg) in 76% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.35 (m, 6H), 7.27 (h, *J* = 6.8 Hz, 12H), 7.16 (d, *J* = 8.6 Hz, 1H), 4.57 (s, 4H), 4.24 (t, *J* = 6.5 Hz, 2H), 3.49 (t, *J* = 6.5 Hz, 2H), 2.41 (s, 3H), 1.25 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.78, 166.62, 150.89, 148.89, 144.16, 138.24, 137.72, 137.52, 132.16, 131.19, 130.13, 129.28, 128.99, 128.58, 128.18, 127.98, 127.86, 127.34, 127.12, 125.76, 118.00, 84.06, 56.52, 47.45, 31.51, 27.89, 21.68. IR (neat): 3029, 2984, 2937, 1639, 1497, 1368, 1154, 811, 738. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{42}H_{41}N_3O_6SNa]^+$, 738.2608; found 738.2567.

4-(((tert-Butyldimethylsilyl)oxy)methyl)-7-(dibenzylamino)-2-phenylisoindoline-1,3-dione (2k)

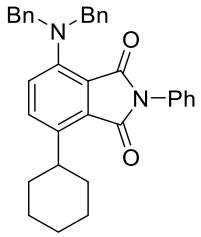


2k

Compound **2k** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (10 mol%), NaBARF (20 mol%) and Boc_2O (2 equiv.) to give **2k** (65.8 mg) in 78% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.80 (dd, *J* =

8.7, 1.6 Hz, 1H), 7.54 – 7.44 (m, 4H), 7.40 (dd, *J* = 7.2, 1.4 Hz, 1H), 7.34 – 7.21 (m, 11H), 5.23 (d, *J* = 1.6 Hz, 2H), 4.61 (s, 4H), 0.98 (d, *J* = 1.7 Hz, 9H), 0.15 (d, *J* = 1.7 Hz, 6H).^{13}C NMR (126 MHz, $CDCl_3$) δ 167.74, 166.78, 148.57, 137.81, 133.76, 133.30, 132.06, 129.10, 128.61, 128.38, 128.14, 128.14, 127.96, 127.37, 126.99, 126.04, 117.23, 60.70, 56.63, 26.12, 18.55, -5.22. IR (neat): 3060, 2849, 1701, 1689, 1494, 1376, 762, 739, 692. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{35}H_{38}N_2O_3SiNa]^+$, 585.2544, found 585.2527.

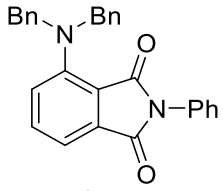
4-Cyclohexyl-7-(dibenzylamino)-2-phenylisoindoline-1,3-dione (2l)



2l

Compound **2l** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2l** (62.3 mg) in 83% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.52 – 7.18 (m, 17H), 4.56 (s, 4H), 3.82 (tt, J = 11.6, 3.3 Hz, 1H), 1.85 (m, 5H), 1.55 – 1.27 (m, 6H). ^{13}C NMR (126 MHz, Chloroform-d) δ 168.06, 166.54, 147.95, 140.74, 137.94, 133.48, 132.16, 129.07, 129.05, 128.56, 128.19, 127.92, 127.31, 127.16, 126.26, 121.08, 118.09, 56.57, 37.45, 33.58, 26.88, 26.36, 26.29, 24.24. IR (neat): 2926, 2851, 1706, 1645, 1498, 1382, 1194, 1118, 884, 737. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{34}H_{33}N_2O_2]^+$, 501.2537; found 501.2523.

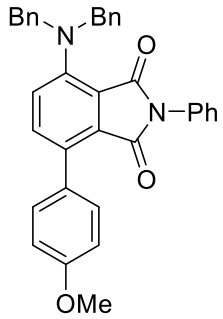
4-(Dibenzylamino)-2-phenylisoindoline-1,3-dione (2m)



2m

Compound **2m** was prepared following general procedure A. The reaction was heated at 80 °C for 24 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2m** (37.6 mg) in 60% yield. ^1H NMR (500 MHz, Chloroform-d) δ 7.54 – 7.15 (m, 18H), 4.64 (s, 4H). ^{13}C NMR (126 MHz, Chloroform-d) δ 167.44, 166.95, 149.73, 137.63, 135.13, 134.73, 132.13, 129.15, 128.66, 128.07, 128.03, 127.45, 127.01, 125.41, 117.04, 115.37, 56.58. IR (neat):2923, 1701, 1612, 1484, 1377, 1112,736, 690. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{28}H_{23}N_2O_2]^+$, 419.1754; found 419.1746.

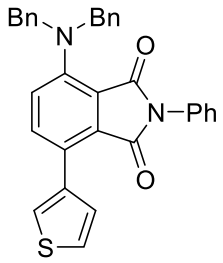
4-(dibenzylamino)-7-(4-methoxyphenyl)-2-phenylisoindoline-1,3-dione (2n)



2n

Compound **2n** was prepared following general procedure A. The reaction was heated at 80 °C for 8 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2n** (70 mg) in 91% yield. ^1H NMR (500 MHz, Chloroform-d) δ 7.46 (m, 7H), 7.33 – 7.20 (m, 12H), 6.99 – 6.88 (m, 2H), 4.62 (s, 4H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, cdcl3) δ 166.99, 166.42, 159.72, 148.71, 137.76, 137.45, 133.17, 132.10, 130.92, 129.05, 128.98, 128.95, 128.66, 128.17, 127.88, 127.44, 127.10, 125.91, 118.28, 113.50, 56.79, 55.41. IR (neat): 1706, 1607, 1376, 1178, 765, 739,692. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{35}H_{28}N_2NaO_3]^+$, 547.1992; found 549.1976.

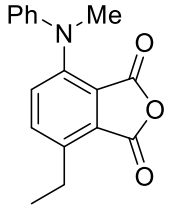
4-(dibenzylamino)-2-phenyl-7-(thiophen-3-yl)isoindoline-1,3-dione (2o)



2o

Compound **2o** was prepared following general procedure A. The reaction was heated at 80 °C for 6 h using **L4AuCl** (5 mol%), NaBARF (10 mol%) and Boc_2O (2 equiv.) to give **2o** (60 mg) in 80% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.62 (dd, J = 3.0, 1.3 Hz, 1H), 7.55 (d, J = 8.7 Hz, 1H), 7.51 – 7.44 (m, 4H), 7.43 – 7.23 (m, 14H), 4.63 (s, 4H). 13C NMR (126 MHz, $CDCl_3$) δ 167.02, 166.35, 148.88, 137.67, 137.19, 137.03, 132.06, 129.27, 129.12, 129.06, 128.68, 128.16, 128.00, 127.72, 127.48, 127.12, 125.98, 124.97, 124.66, 56.82. IR (neat): 3027, 1703, 1597, 1488, 1378, 1119, 734, 690. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{32}H_{24}N_2NaO_2S]^+$, 523.1451; found 523.1459.

4-Ethyl-7-(methyl(phenyl)amino)isobenzofuran-1,3-dione (2f')

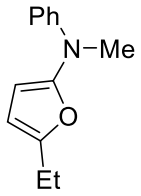


2f'

To a dried, Ar protected schlenk tube were added sequentially 0.15 mmol ynamide **1f**, 0.0075 mmol **L4**AuCl (5 mol%), 0.015 mmol NaBARF (10 mol%) and 3 mL anhydrous DCE as solvent. The reaction was then heated at 80 ^{o}C for 10 h. Maleic anhydride (2 equiv) was added and stirred for 5 h at room temperature. The reaction was concentrated under reduced pressure. The residue was purified through silica gel flash chromatography to give **2f'** (34.6 mg) in 82% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.32 – 7.25 (m, 8H), 7.23 – 7.19 (m, 2H), 7.16 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 4.56 – 4.36 (m, 4H), 4.16 (s, 4H), 2.95 (t, *J* = 6.0 Hz, 2H), 1.35 (t, *J* = 7.2 Hz,

3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.40, 163.31, 148.43, 137.68, 135.50, 135.08, 129.14, 128.75, 128.35, 128.25, 127.23, 123.45, 67.10, 61.99, 57.96, 27.79, 14.01. IR (neat): 3038, 2971, 2934, 1834, 1766, 1597, 1495, 1210, 910, 755. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{17}H_{16}NO_3]^+$, 282.1125; found 282.1132.

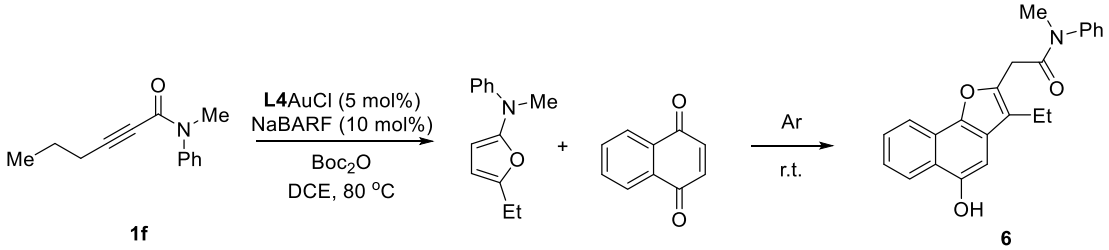
5-ethyl-N-methyl-N-phenylfuran-2-amine (5)



5

To a dried, Ar-protected Schlenk tube were added sequentially 0.15 mmol ynamide **1f**, 0.0075 mmol **L4**AuCl (5 mol%), 0.015 mmol NaBARF (10 mol%) and 3 mL anhydrous DCE as the solvent. The reaction was then heated at 80 °C for 12 h. After cooled to room temperature. 0.05 mmol 1,3,5-trimethoxy benzene solution was injected under Ar as an internal reference. The reaction finished in 12 h, and the NMR yield is 85%. Silica gel was added, and the solvent was removed under vacuum. Silica gel chromatography under Ar afforded the oxygen-sensitive furan intermediate **5** in about 30% isolated yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.23 (t, J = 7.5 Hz, 2H), 6.87 – 6.81 (m, 3H), 5.95 (d, J = 1.8 Hz, 1H), 5.78 (d, J = 3.1 Hz, 1H), 3.25 (s, 3H), 2.60 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.00, 152.67, 148.11, 129.04, 119.44, 114.95, 104.78, 99.32, 39.17, 21.65, 12.24. 2D NMR COSY, HSQC and HMBC are also attached. IR (neat): 2920, 1498, 1127, 749, 691, 497. MS-ESI (m/z): $[M+H]^+$ calcd. for [C13H16NO]$^+$,202.1226; found 202.1232.

2-(3-Ethyl-5-hydroxynaphtho[1,2-*b*]furan-2-yl)-*N*-methyl-*N*-phenylacetamide (6)



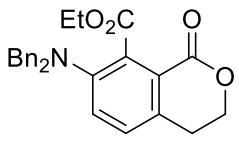
1f **6**

To a dried, Ar protected schlenk tube were added sequentially 0.15 mmol ynamide **1f**, 0.0075 mmol **L4**AuCl (5 mol%), 0.015 mmol NaBARF (10 mol%), Boc_2O and 3 mL anhydrous DCE. The reaction was heated at the 80 ^oC for 12 h, The reaction was cooled to room temperature, 0.30 mmol naphthalene-1,4-dione (2 equiv.) was added under Ar atmosphere. After 2 more hours at room temperature. The reaction was concentrated under reduced pressure. The residue was purified through silica gel flash chromatography to give **6** (45.8 mg) in 85% yield. ^1H NMR (500 MHz, Chloroform-d) δ 8.18 (d, J = 8.3 Hz, 1H), 8.00 (d, J = 8.1 Hz, 1H), 7.52 – 7.30 (m, 8H), 6.55 (s, 1H), 3.65 (s, 2H), 3.41 (s, 3H), 2.15 (q, J = 7.6 Hz, 2H), 0.97 (t, J = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 169.87, 147.91, 145.41, 144.36, 143.74, 130.11, 128.38, 127.56, 126.05, 123.78, 123.68, 123.08, 122.96, 121.33, 120.30, 119.71, 38.22, 32.70, 16.70, 14.60. IR (neat): 3269 (broad peak), 2965, 1634, 1421, 1247, 1223, 1125, 1071, 765, 699, 557. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{23}H_{21}NNaO_3]^+$,382.1414; found 382.1415.

Gold catalyzed intramolecular ynamide isomerization and D-A reactions

General procedure B: To a dried, Ar protected Schlenk tube were added sequentially 0.15 mmol ynamide **7**, 0.0075-0.0150 mmol **L4**AuCl (5-10 mol%), 0.015-0.030 mmol NaBARF (10-20 mol%), Boc_2O (2equiv.) and 3 mL anhydrous DCE as the solvent. The reaction was then heated at the 80 ^oC for 24 h and monitored by TLC or NMR. The reaction was concentrated under reduced pressure. The residue was purified through silica gel flash chromatography to obtain pure product **8**.

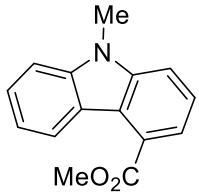
7-(Dibenzylamino)-8-ethylisochroman-1-one (8a)



8a

Compound **8a** was prepared following general procedure B. The reaction was heated at 80 °C for 24 h using **L4AuCl** (10 mol%), NaBARF (20 mol%) and Boc_2O (2 equiv.) to give **8a** (46.7 mg) in 75% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.31 – 7.26 (m, 8H), 7.21 (t, *J* = 6.7 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 4.50 – 4.45 (m, 4H), 4.16 (s, 4H), 2.95 (t, *J* = 6.0 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.40, 163.31, 148.43, 137.68, 135.50, 135.08, 129.14, 128.75, 128.35, 128.25, 127.23, 123.45, 67.10, 61.99, 57.96, 27.79, 14.01. IR (neat): 3063, 3029, 2984, 1728, 1632, 1495, 1283, 1127, 1027, 961, 742. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{26}H_{26}NO_4]^+$, 416.1856; found 416.1861.

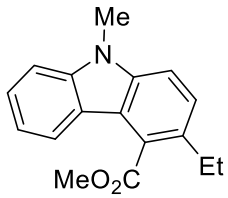
Methyl 9-methyl-9H-carbazole-4-carboxylate (8b)



8b

Compound **8b** was prepared following general procedure B. The reaction was heated at 80 °C for 24 h using **L4AuCl** (5 mol%) and NaBARF (10 mol%) to give **8b** (32.3 mg) in 90% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.89 (dt, J = 8.2, 1.0 Hz, 1H), 7.87 (dd, J = 7.5, 1.0 Hz, 1H), 7.60 (dd, J = 8.3, 1.0 Hz, 1H), 7.54 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.50 (dd, J = 8.2, 7.5 Hz, 1H), 7.42 (dt, J = 8.3, 0.9 Hz, 1H), 7.29 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 4.08 (s, 3H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 168.59, 141.84, 141.78, 126.83, 125.74, 125.37, 124.68, 122.21, 121.49, 121.48, 119.39, 112.74, 108.33, 52.26, 29.27. IR (neat): 2921, 1711, 1439, 1255, 1074, 742, 719. MS-ESI (*m/z*): $[M+H]^+$ calcd. for $[C_{15}H_{14}NO_2]^+$, 240.1019; found 240.1038.

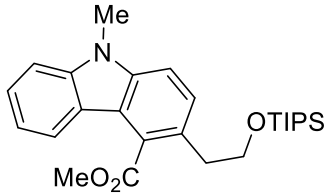
Methyl 3-ethyl-9-methyl-9H-carbazole-4-carboxylate (8c)



8c

Compound **8c** was prepared following general procedure B. The reaction was heated at 80 °C for 24 h using **L4AuCl** (5 mol%) and NaBARF (10 mol%) to give **8c** (44.8 mg) in 90% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.92 (dt, J = 8.0, 1.2 Hz, 1H), 7.48 (ddd, J = 8.2, 7.1, 1.2 Hz, 1H), 7.41 – 7.30 (m, 3H), 7.21 (ddd, J = 8.1, 7.1, 1.1 Hz, 1H), 4.12 (s, 3H), 3.80 (s, 3H), 2.84 (q, J = 7.6 Hz, 2H), 1.32 (t, J = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-d) δ 170.64, 141.55, 139.51, 132.27, 126.63, 126.12, 125.73, 121.64, 121.03, 119.21, 119.15, 110.24, 108.66, 52.37, 29.18, 26.75, 16.84. IR (neat): 2962, 1716, 1467, 1253, 1086, 818, 744, 725. MS-ESI (*m/z*): $[M+Na]^+$ calcd. for $[C_{17}H_{17}NNaO_2]^+$, 290.1151; found 290.1167.

Methyl 9-methyl-3-(2-((triisopropylsilyl)oxy)ethyl)-9H-carbazole-4-carboxylate (8d)



8d

Compound **8d** was prepared following general procedure B. The reaction was heated at 80 °C for 24 h using **L4AuCl** (10 mol%) and NaBARF (20 mol%) to give **8d** (64.6 mg) in 98% yield. ^{1}H NMR (600 MHz, Chloroform-d) δ 7.90 (d, J = 7.9 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.43 – 7.37 (m, 3H), 7.23 – 7.19 (m, 1H), 4.11 (s, 3H), 3.94 (t, J = 7.5 Hz, 2H), 3.83 (s, 3H), 3.07 (t, J = 7.5 Hz, 2H), 1.19 – 0.95 (m, 21H). ^{13}C NMR (151 MHz, Chloroform-d) δ 170.44, 141.52, 139.82, 128.30, 126.84, 126.57, 126.18, 121.66, 121.04, 119.28, 119.24, 109.96, 108.70, 65.24, 52.46, 37.40, 29.23, 18.16, 12.13. IR (neat): 2944, 2865, 1720, 1465, 1257, 1091, 882, 816, 741, 683, 641. MS-ESI (m/z): [M+Na]+ calcd. for $[C_{26}H_{37}NNaO_3Si]$+, 462.2435; found 462.2444.

References

[1] Y.Yasui, S. Tsuchida, H. Miyabe, Y. Takemoto, *J. Org. Chem.*, **2007**, *72*, 5898-5900;

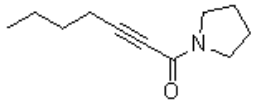
[2] J. F. Teichert, S. Zhang, A. W. van Zijl, J. W. Slaa, A. J. Minnaard, B. L. Feringa, *Org. Lett.*, **2010**, *12*, 4658-4660;

[3] A. Martinez-Cuezva, C. Lopez-Leonardo, D. Bautista, M. Alajarin, and J. Berna, *J. Am. Chem. Soc.*, **2016**, *138*, 8726-8729;

[4] Christine M. Le, Theresa Sperger, Rui Fu, Xiao Hou, Yong Hwan Lim, Franziska Schoenebeck, Mark Lautens, *J. Am. Chem. Soc.*, **2016**, 138, 14441-14448;

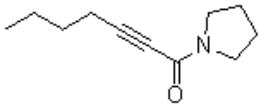
xg-2-182A-h

Parameter	Value
1 Title	xg-2-182A-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

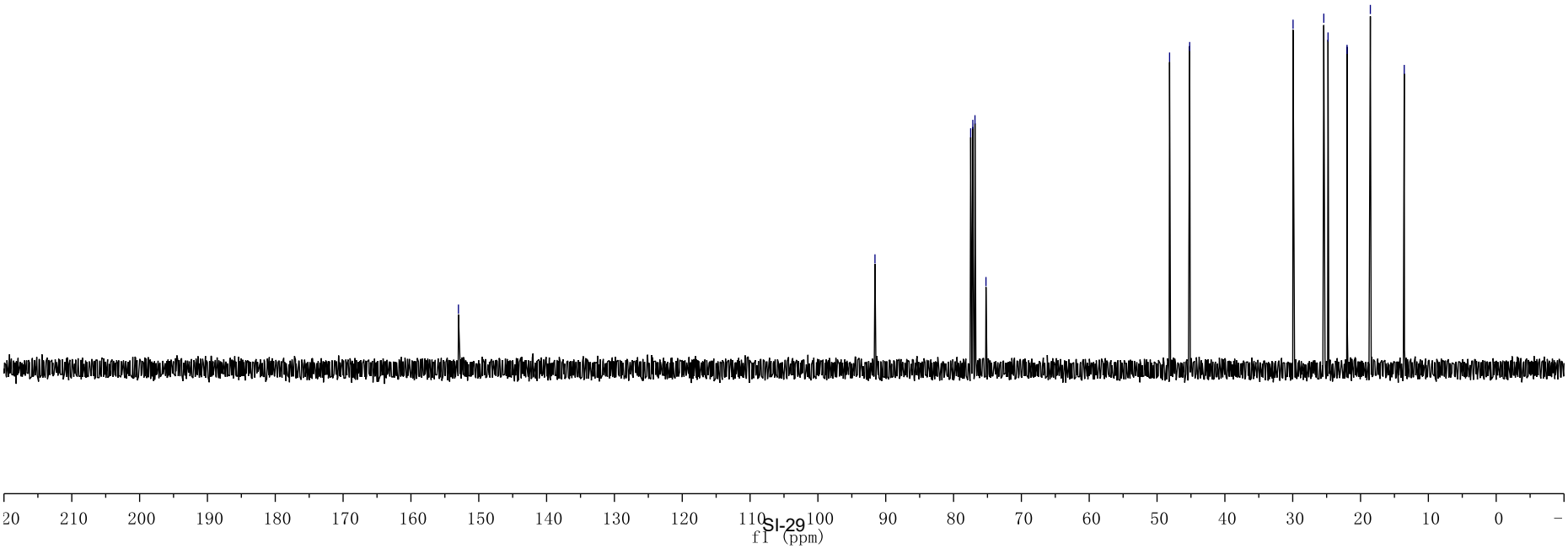


xg-2-182A-c13

Parameter	Value
1 Title	xg-2-182A-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C

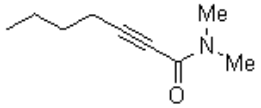


153.00
91.59
77.48
77.16
76.84
75.22
48.15
45.19
29.95
25.42
24.79
21.99
18.55
13.55



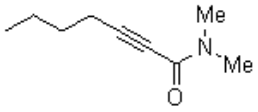
xg-2-204A-h

Parameter	Value
1 Title	xg-2-204A-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

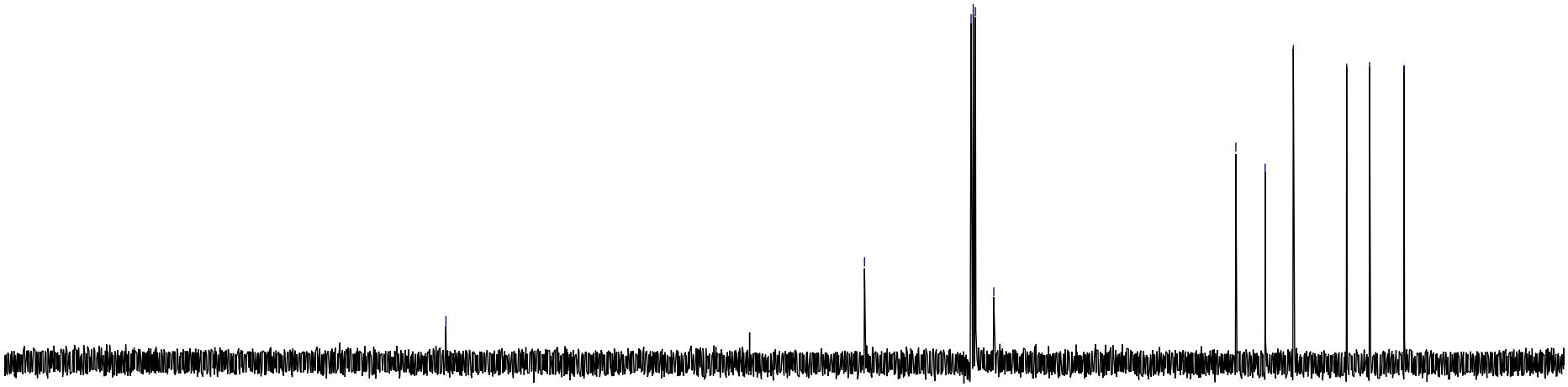


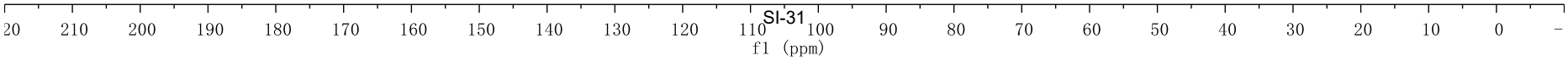
xg-2-204A-c13

Parameter	Value
1 Title	xg-2-204A-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



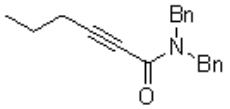
154.92
93.19
77.48
77.16
76.84
74.13
38.43
34.11
29.95
22.09
18.70
13.60





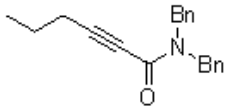
xg-2-192B-h

Parameter	Value
1 Title	xg-2-192B-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H



xg-2-192B-c13

Parameter	Value
1 Title	xg-2-192B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



155.31
136.54
136.39
128.94
128.78
128.58
127.99
127.81
127.70
93.90
77.48
77.16
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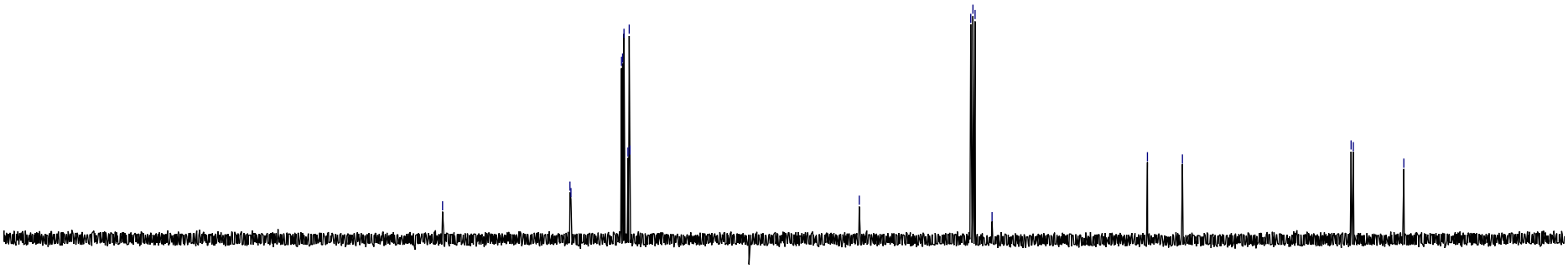
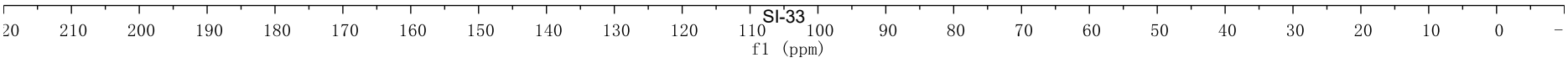
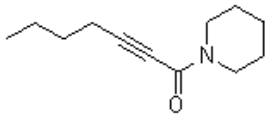
74.34
51.45
46.29
21.44
21.11
13.67





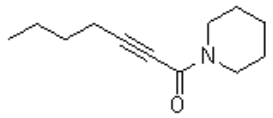
xg-2-200C

Parameter	Value
1 Title	xg-2-200C
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

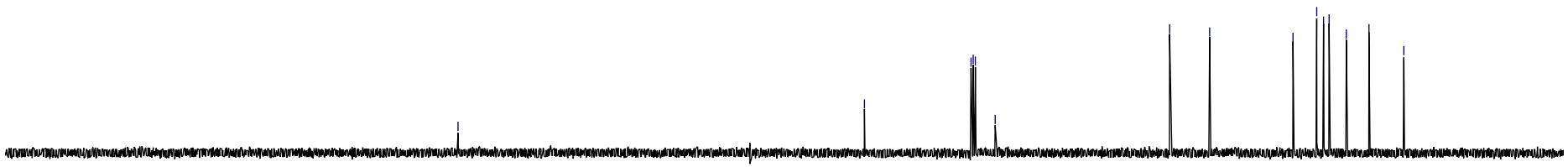


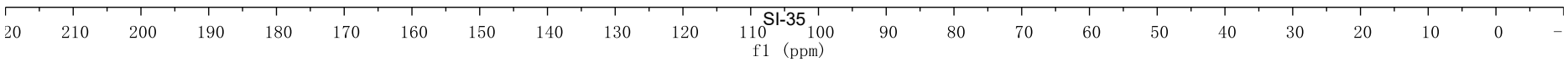
xg-2-200C-c13

Parameter	Value
1 Title	xg-2-200C-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



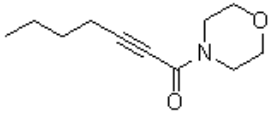
153.20
93.21
77.48
77.16
76.84
73.91
48.16
42.26
29.95
26.46
25.44
24.63
22.09
18.75
13.60





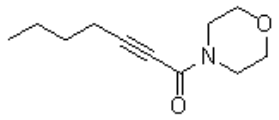
xg-2-200B

Parameter	Value
1 Title	xg-2-200B
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

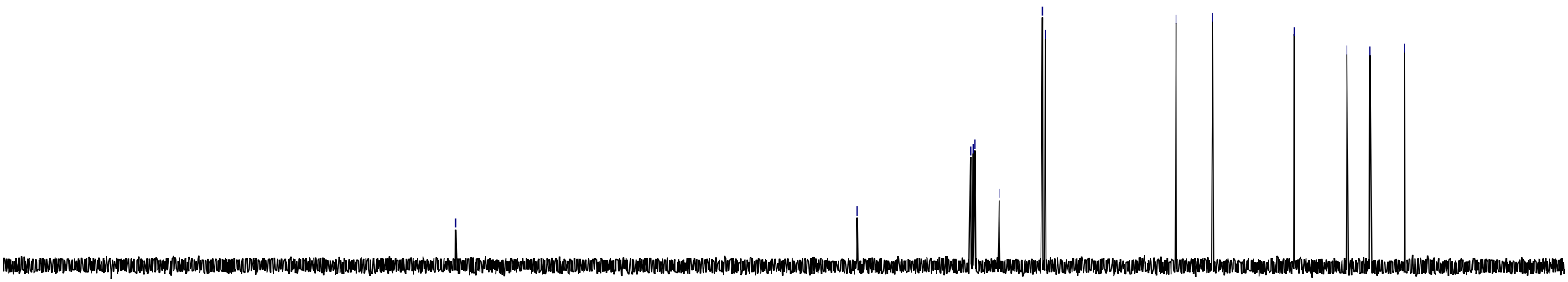


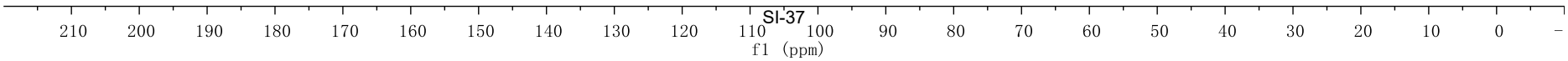
xg-2-200B-c13

Parameter	Value
1 Title	xg-2-200B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



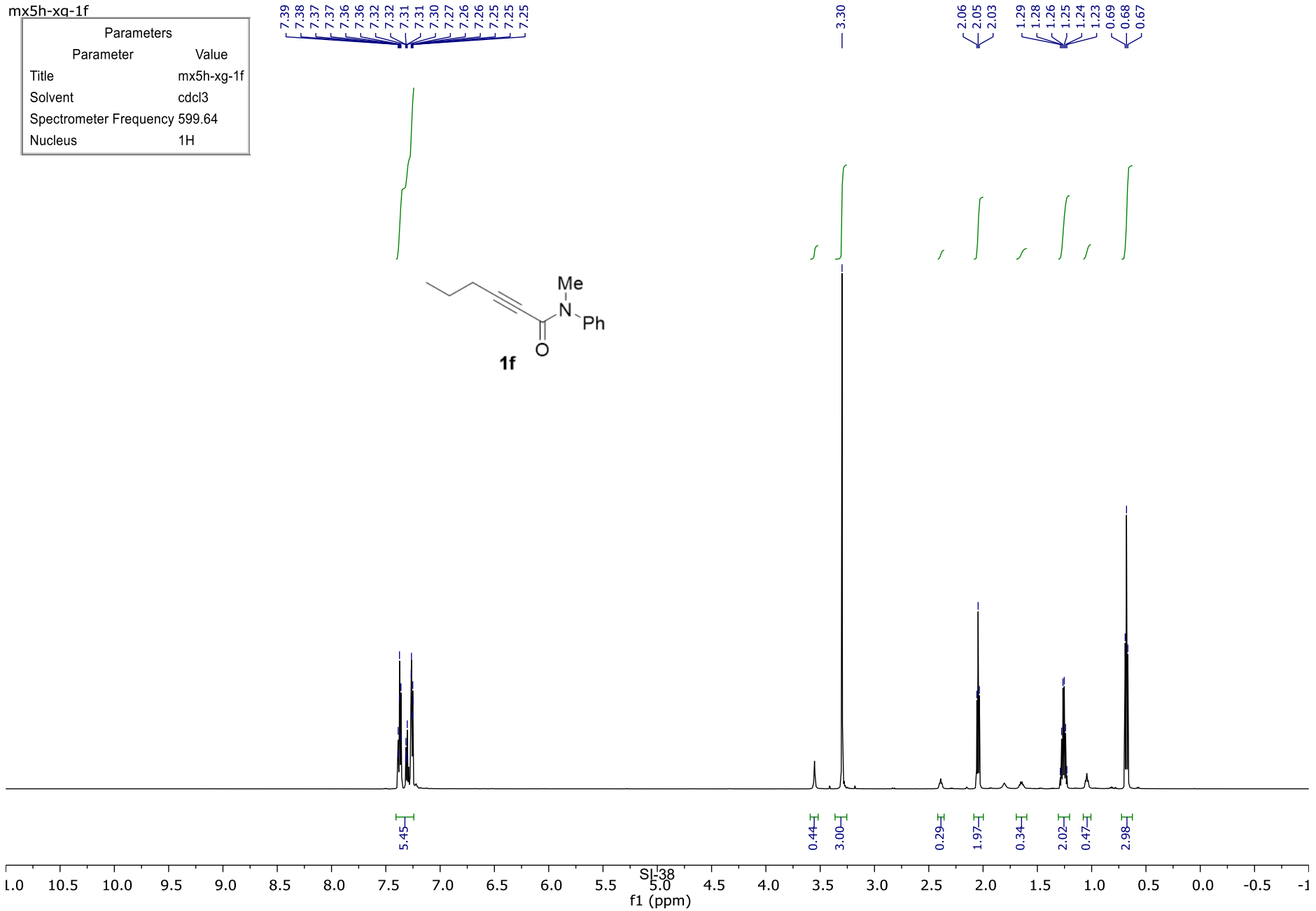
153.36
94.23
77.48
77.16
76.84
73.29
66.89
66.49
47.23
41.83
29.82
22.05
18.66
13.53





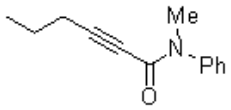
mx5h-xg-1f

Parameters	
Parameter	Value
Title	mx5h-xg-1f
Solvent	cdcl3
Spectrometer Frequency	599.64
Nucleus	1H

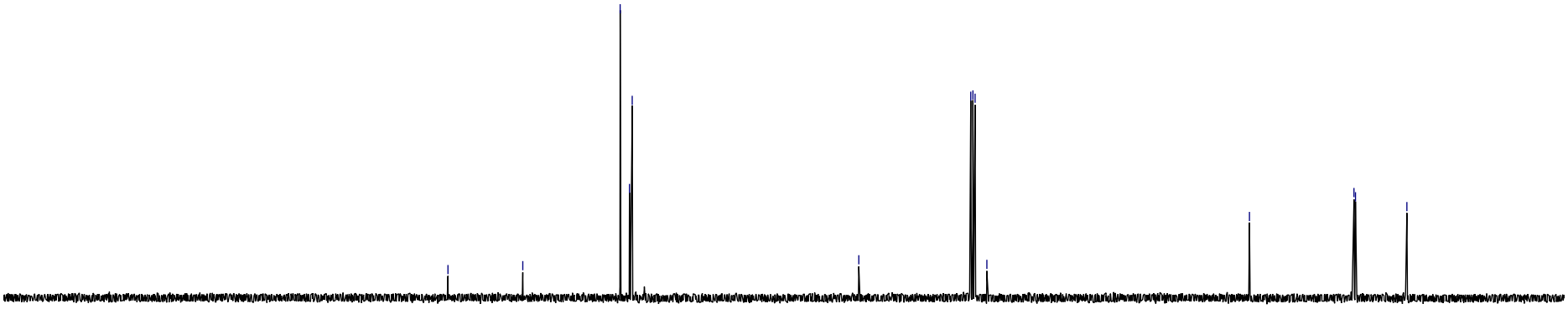


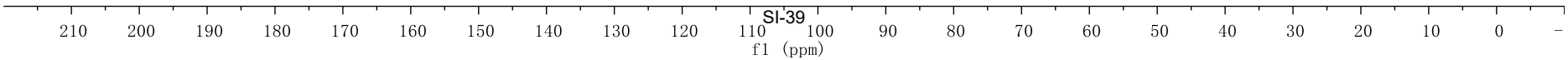
xg-2-195A-c13

Parameter	Value
1 Title	xg-2-195A-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



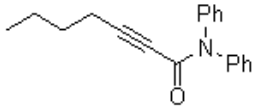
154.52
143.49
129.14
127.77
127.36
93.98
77.48
77.16
76.84
75.11
36.41
21.01
20.79
13.22





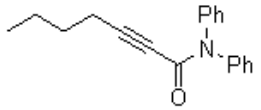
xg-2-194B

Parameter	Value
1 Title	xg-2-194B
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

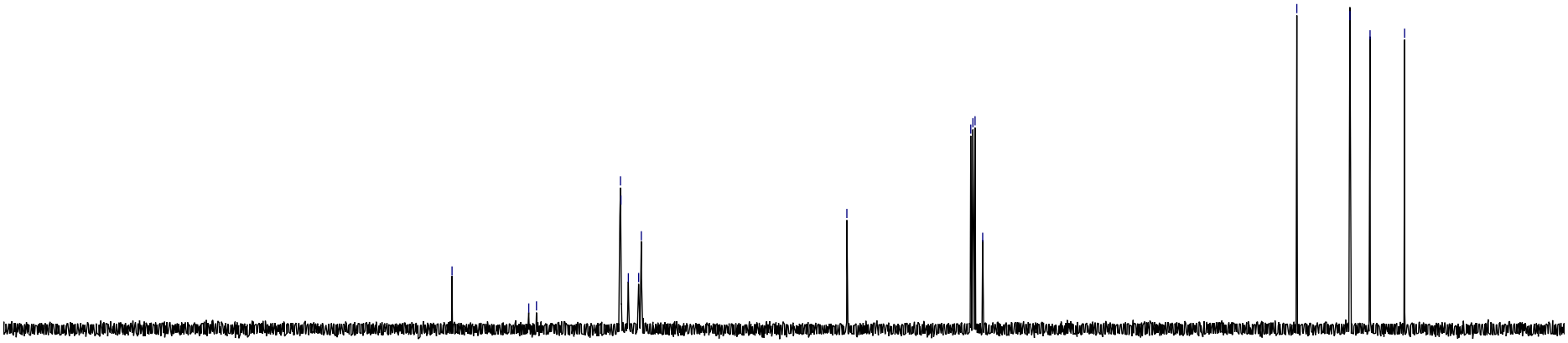


xg-2-194B-c13

Parameter	Value
1 Title	xg-2-194B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



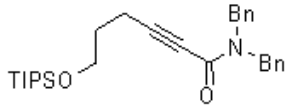
153.91
142.61
141.47
129.09
129.02
127.93
126.42
126.02
95.74
77.48
77.16
76.84
75.72
29.43
21.61
18.64
13.55



f1 (ppm)

xg-2-224A-h

Parameter	Value
1 Title	xg-2-224A-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



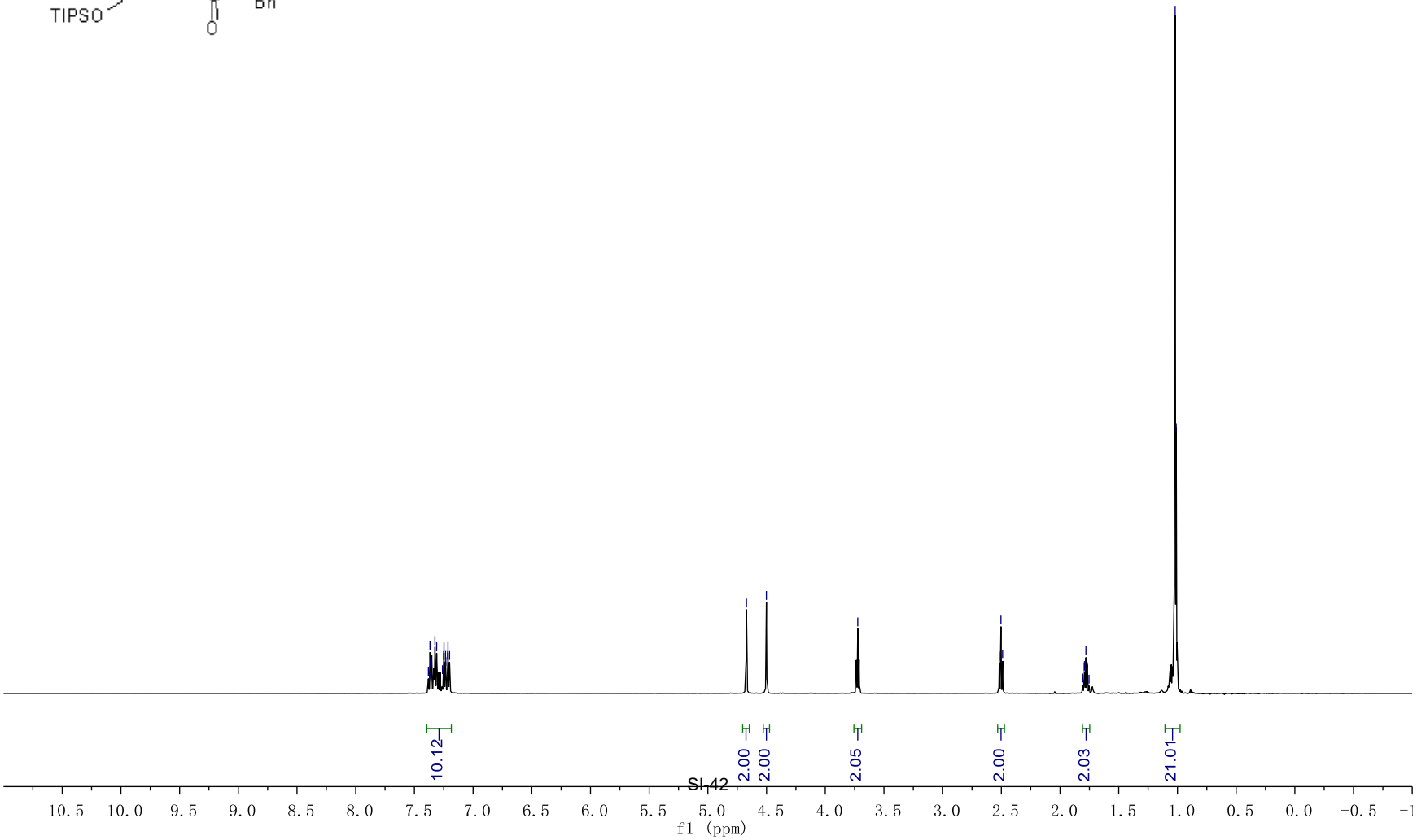
7.38 7.37 7.37 7.36 7.32 7.31 7.26 7.25 7.25 7.23 7.23 7.22 7.21 7.20

4.67 4.50

3.72

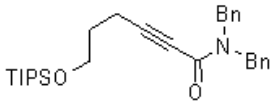
2.52 2.50 2.49 1.81 1.79 1.79 1.78 1.77 1.77 1.75

1.02 1.01



xg-2-224A-c13

Parameter	Value
1 Title	xg-2-224A-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



155.21
136.49
136.32
128.91
128.74
128.52
127.96
127.75
127.66
93.80
77.41
77.16
76.91
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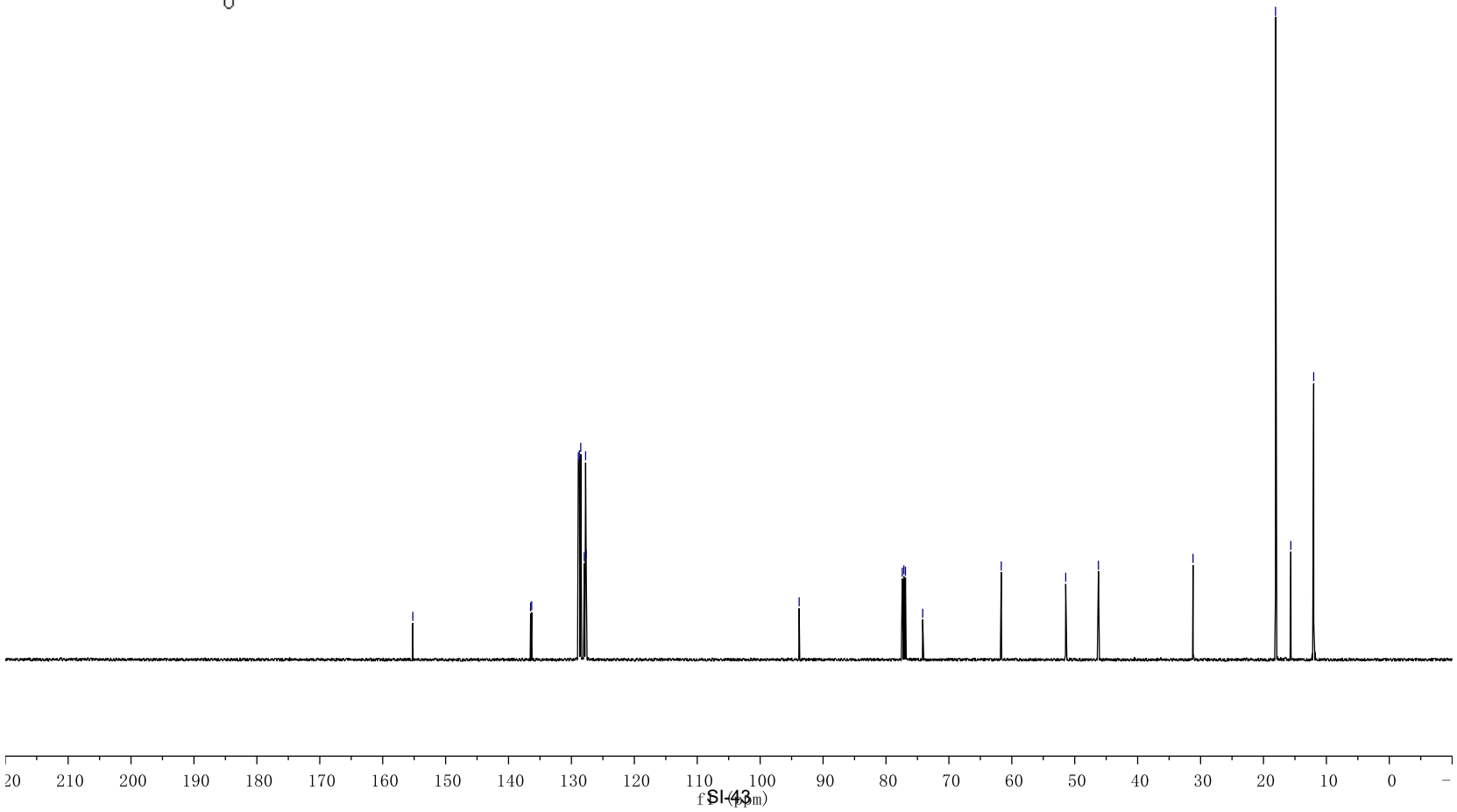
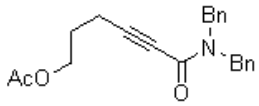
51.43
46.23
31.19
18.08
15.65
12.02



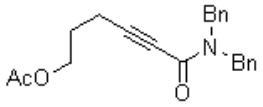
xg-3-34B-h

Parameter	Value
1 Title	xg-3-34B-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H



xg-3-34B-c13

Parameter	Value
1 Title	xg-3-34B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



170.30
154.84
136.23
136.08
128.80
128.62
128.39
127.85
127.57
127.51
92.01
77.38
77.06
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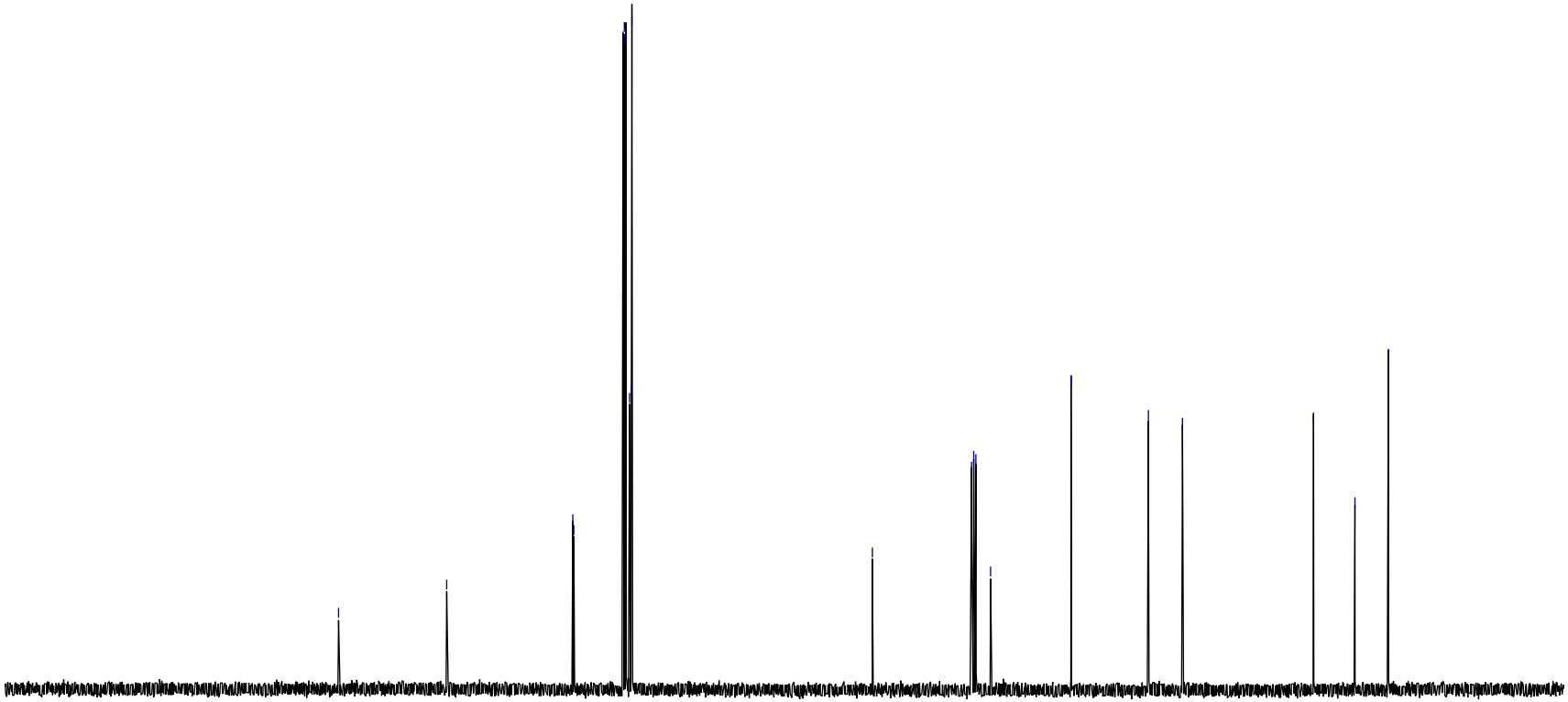
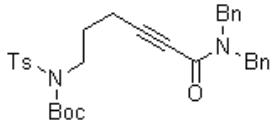
62.70
51.28
46.25
26.90
20.80
15.86



f1 (ppm)

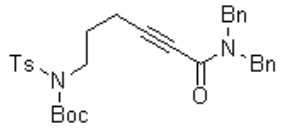
xg-2-228B-h

Parameter	Value
1 Title	xg-2-228B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



xg-2-228B-c13

Parameter	Value
1 Title	xg-2-228B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



154.91
150.74
144.22
137.11
136.29
136.23
129.26
128.78
128.62
128.37
127.79
127.72
127.68
127.54
92.13
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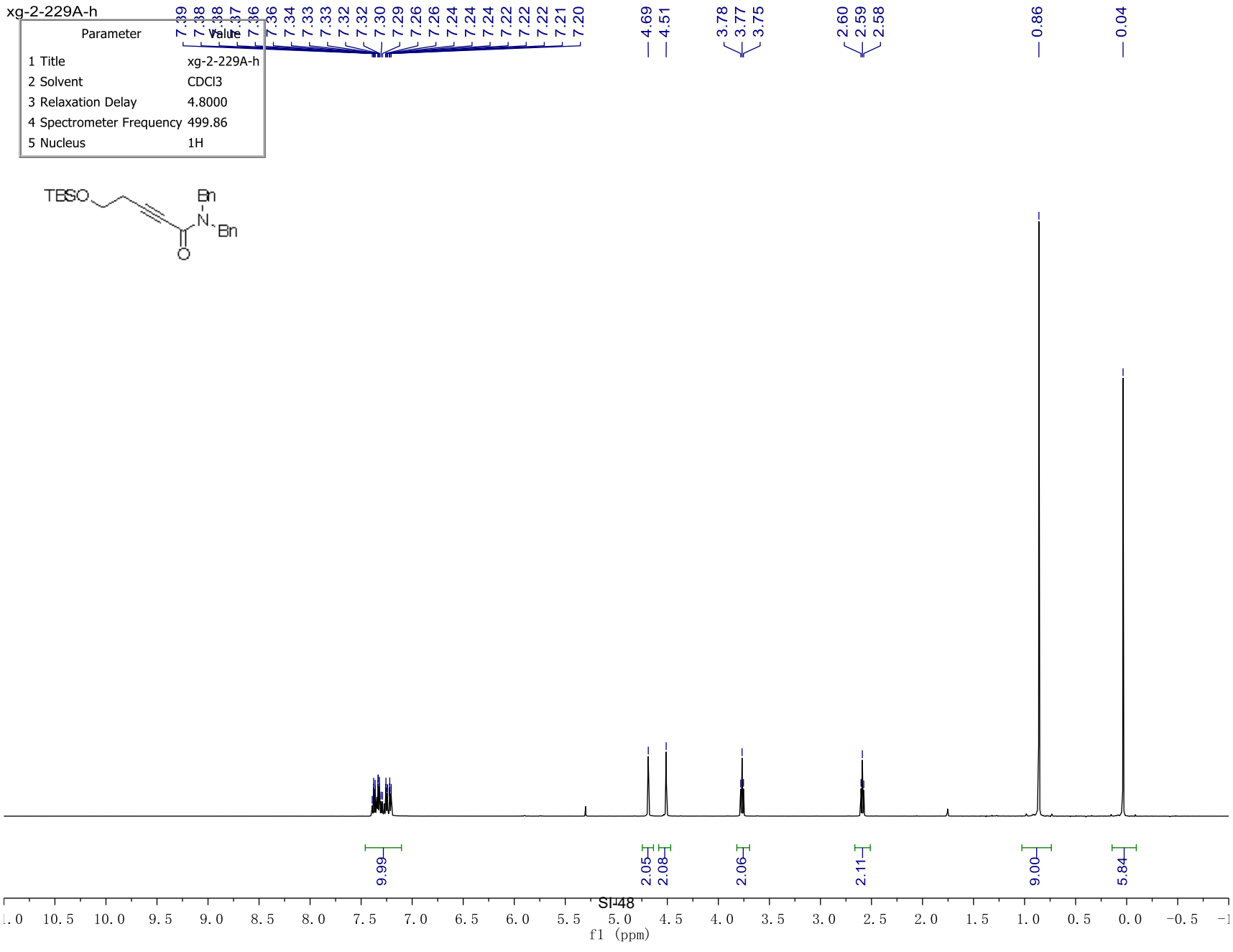
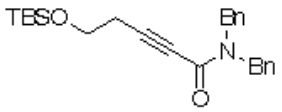
46.20
46.13
28.29
27.82
21.58
16.60

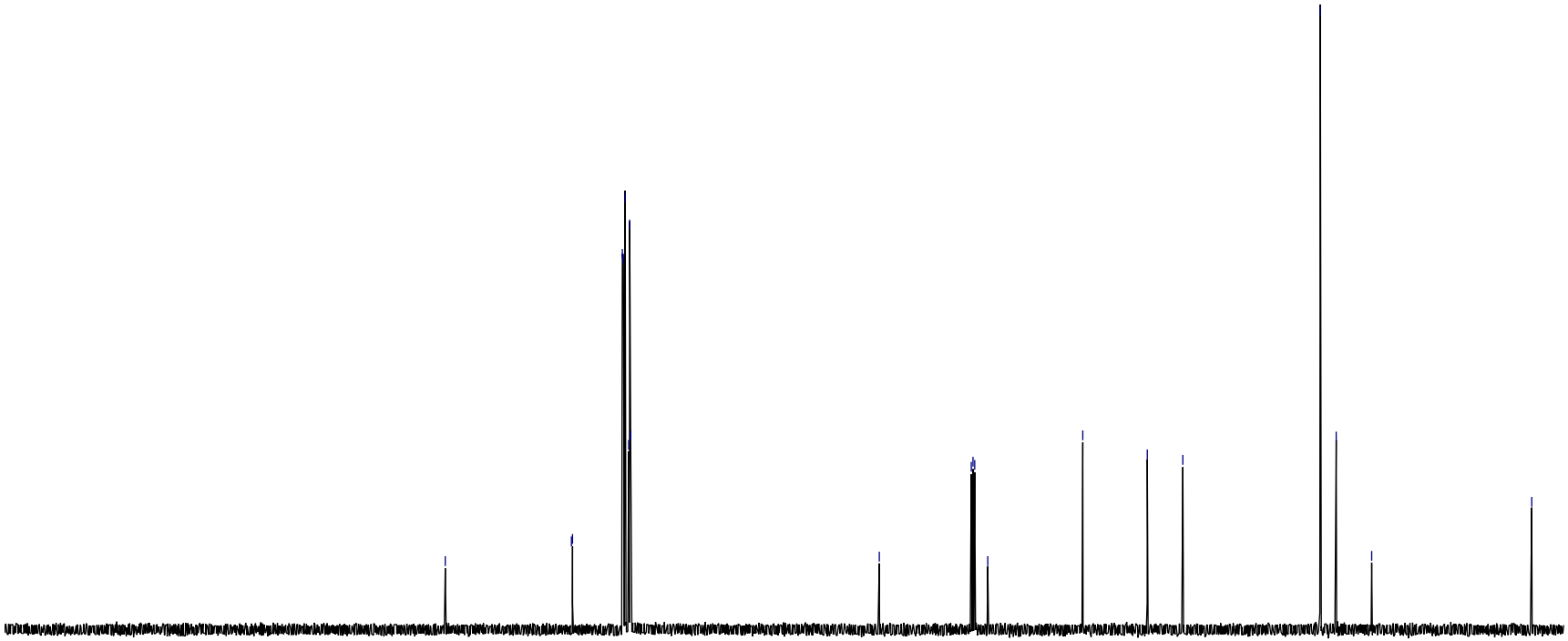

xg-2-229A-h
Parameter Value
1 Title xg-2-229A-h
2 Solvent CDCl3
3 Relaxation Delay 4.8000
4 Spectrometer Frequency 499.86
5 Nucleus 1H
TBSO
Bn
N
Bn
O
7.39 7.38 7.38 7.37 7.36 7.36 7.34 7.33 7.33 7.32 7.32 7.30 7.29 7.26 7.26 7.24 7.24 7.24 7.22 7.22 7.22 7.21 7.20
4.69 4.51
3.78 3.77 3.75
2.60 2.59 2.58
0.86
0.04
9.99 2.05 2.08 2.06 2.11 9.00 5.84
f1 (ppm)

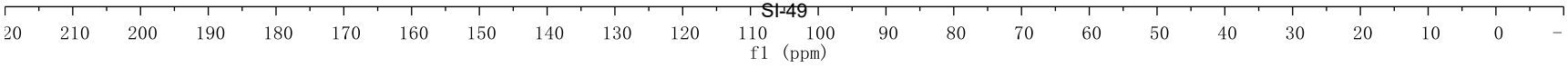
xg-2-229A-c13

Parameter	Value
1 Title	xg-2-229A-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



155.03
136.41
136.25
128.90
128.75
128.49
127.97
127.82
127.67
90.99
77.42
77.16
76.91
74.98
60.96
51.44
46.20
25.91
23.56
18.33
-5.29

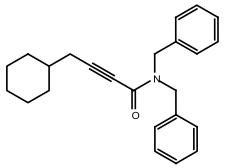


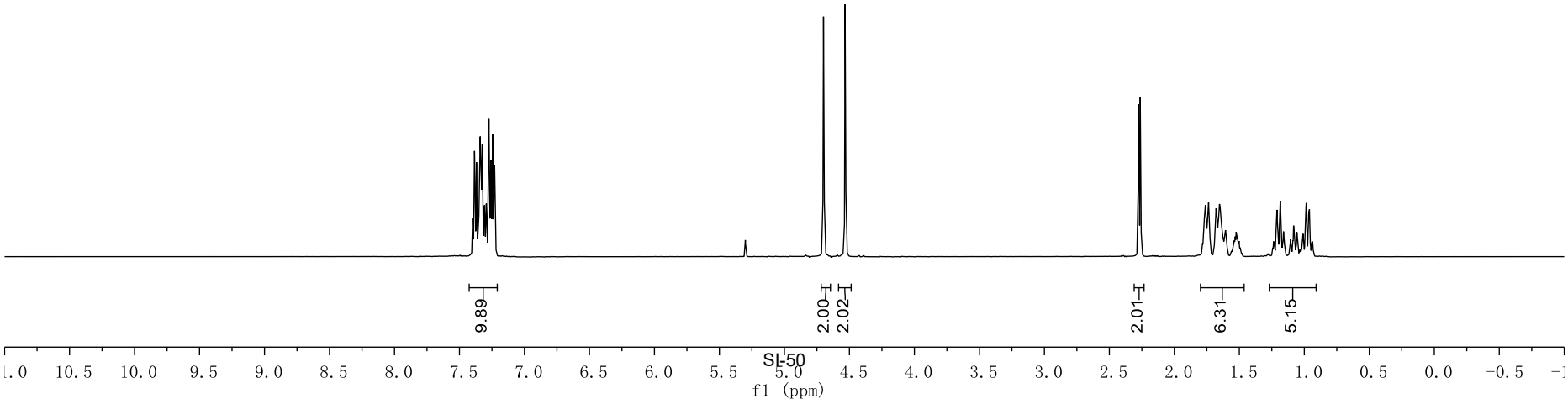


mx4h-189-Cy

Parameters

Parameter	Value
Title	mx4h-189-Cy
Author	vnmr1
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H

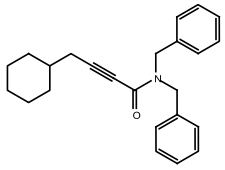


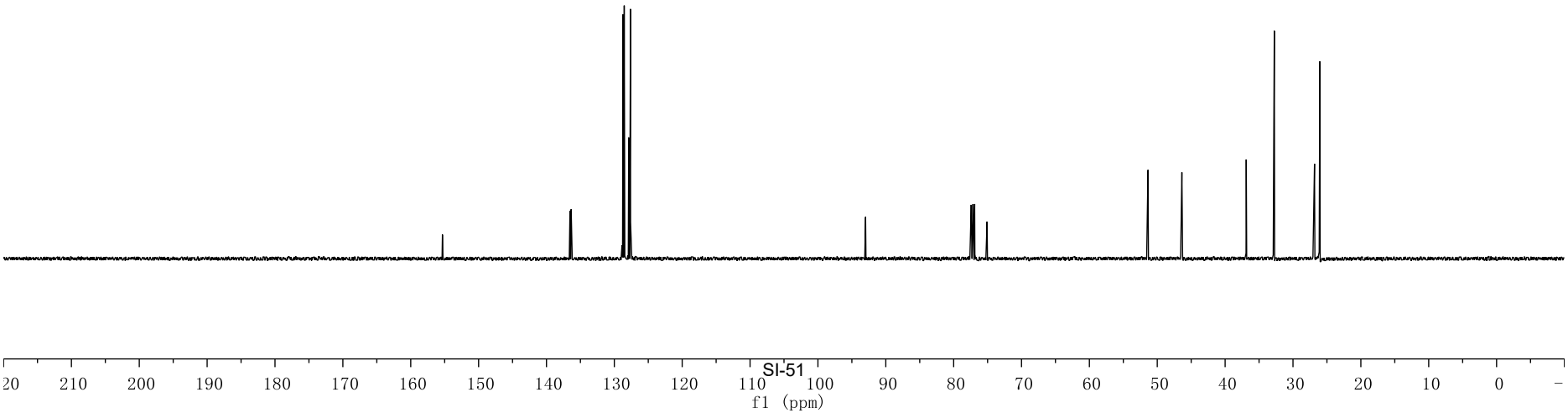


mx4c-189-Cy1

Parameters	
Parameter	Value
Title	mx4c-189-Cy1
Author	
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

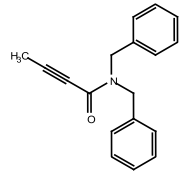
155.33
136.54
136.36
128.86
128.72
128.54
127.88
127.64
127.62
92.98
75.07
51.37
46.37
36.89
32.75
26.83
26.07
26.05

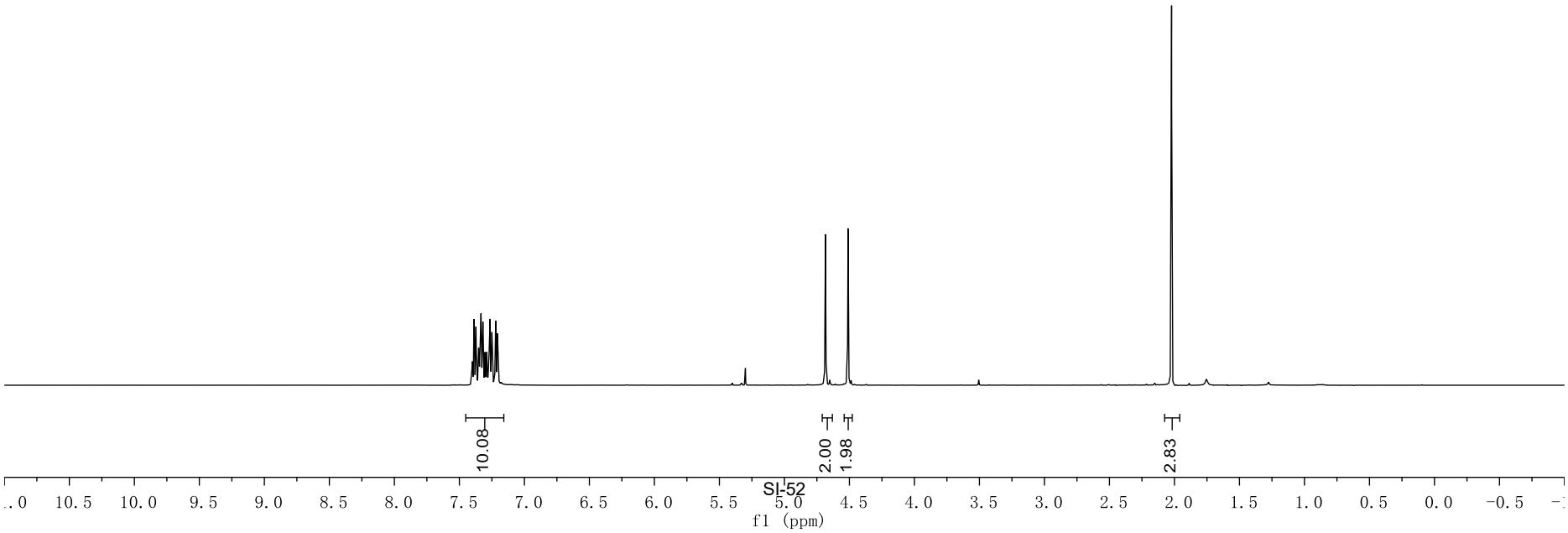




mx4h-189-1m

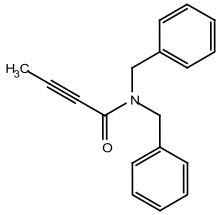

7.40
7.39
7.39
7.38
7.38
7.37
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.32
7.31
7.30
7.30
7.29
7.27
7.27
7.26
7.25
7.25
7.25
7.22
7.22
7.22
7.21
7.21
7.20
4.68
4.51
2.02


H3C
N
O

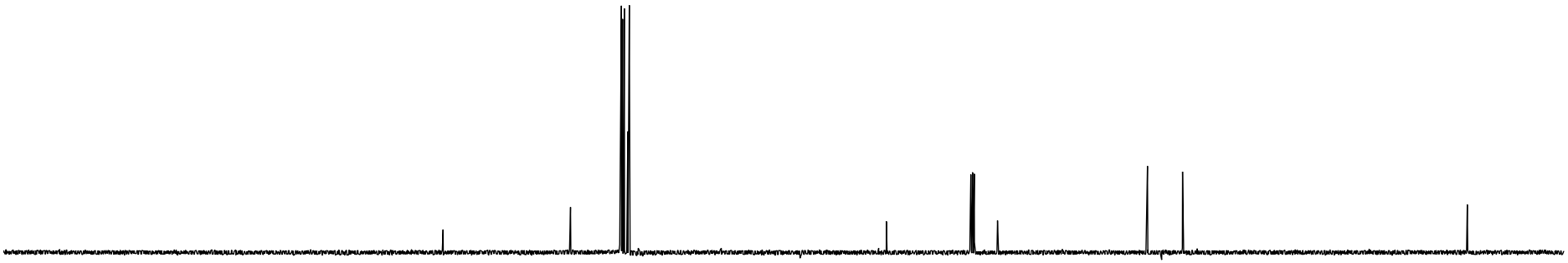

10.08
2.00
1.98
2.83
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

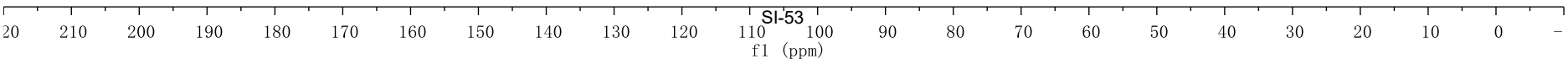
mx4c-189-1m

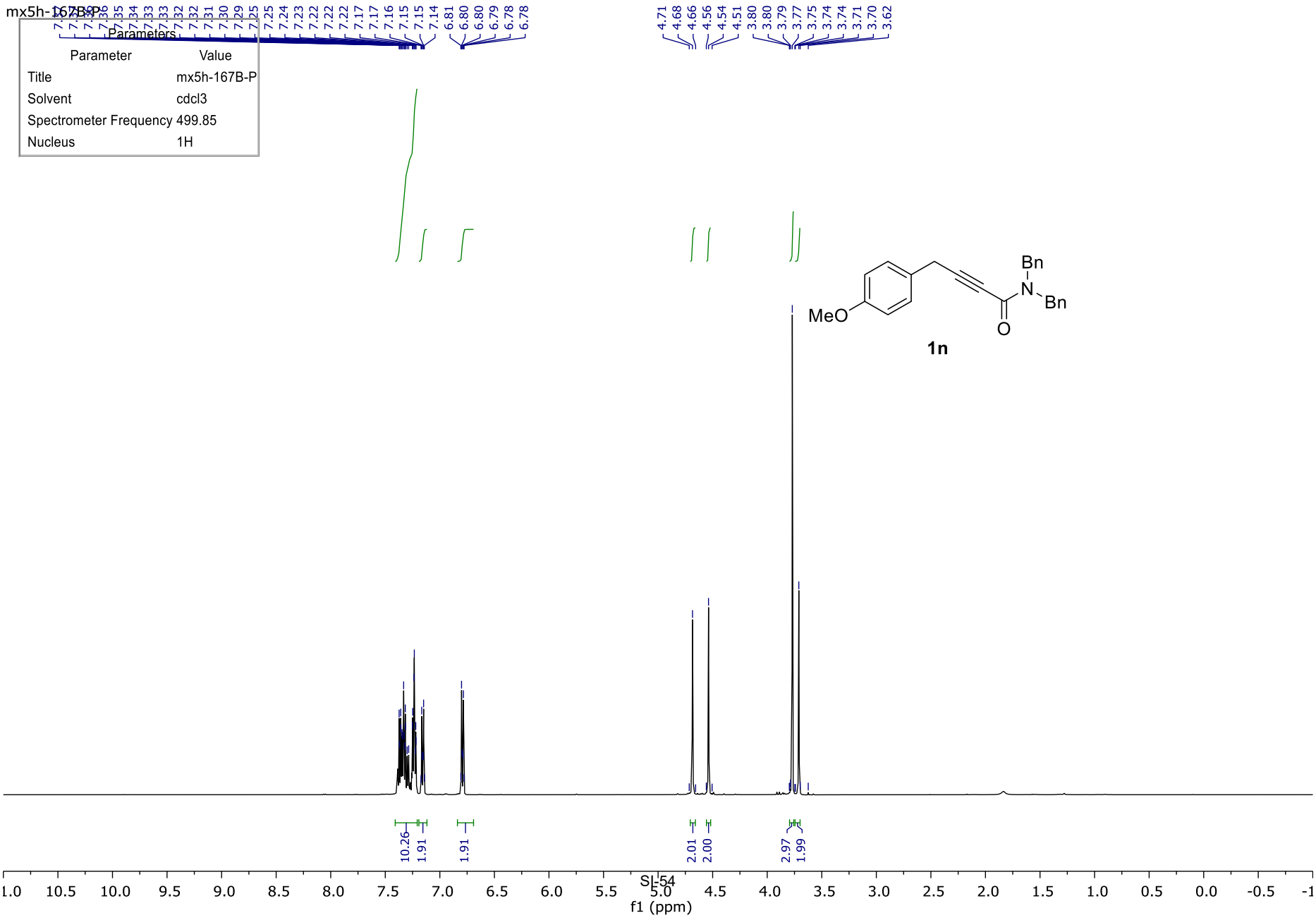
Parameters	
Parameter	Value
Title	mx4c-189-1m
Author	
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C



155.20
136.42
136.30
128.92
128.75
128.49
127.98
127.76
127.67
89.86
77.41
77.16
76.91
73.48
51.37
46.20
4.23



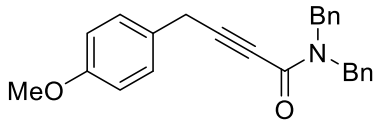



mx5h-167B-P
Parameters
Parameter Value
Title mx5h-167B-P
Solvent cdcl3
Spectrometer Frequency 499.85
Nucleus 1H
7.36 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.29 7.25 7.25 7.24 7.23 7.22 7.22 7.22 7.17 7.17 7.16 7.15 7.15 7.14 6.81 6.80 6.80 6.79 6.78 6.78
4.71 4.68 4.66 4.56 4.54 4.51 3.80 3.80 3.79 3.77 3.75 3.74 3.74 3.71 3.70 3.62
MeO
Bn
N
Bn
O
1n
10.26 1.91 1.91 2.01 2.00 2.97 1.99
f1 (ppm)

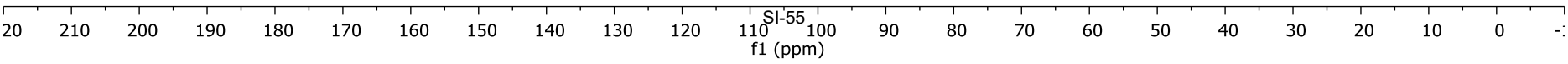
mx5c-167B-P
Std carbon

Parameters	
Parameter	Value
Title	mx5c-167B-P
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

158.69
155.07
136.38
136.22
129.01
128.90
128.83
128.74
128.58
128.52
127.94
127.69
127.65
127.36
126.62
114.19
91.40
75.69
55.36
51.39
46.44
24.61



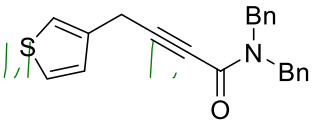
1n



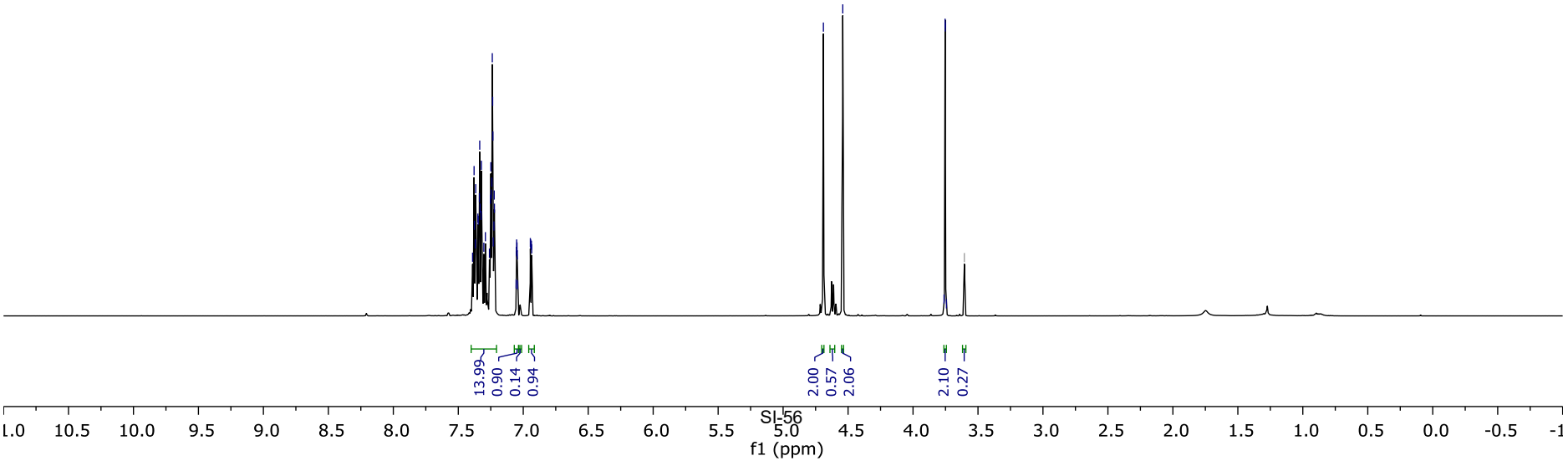
mx5h-178A-PFinal

Parameters	
Parameter	Value
Title	mx5h-178A-PFinal
Solvent	cdcl3
Spectrometer Frequency	599.64
Nucleus	1H

7.39 7.38 7.38 7.37 7.37 7.35 7.34 7.34 7.33 7.32 7.32 7.30 7.29 7.26 7.25 7.25 7.25 7.24 7.24 7.24 7.23 7.23 7.23 7.22 7.22 7.05 7.05 7.05 7.05 7.04 6.95 6.94 6.94 6.93 4.69 4.54 3.76 3.75 3.75 3.74 3.61 inpurities



1o

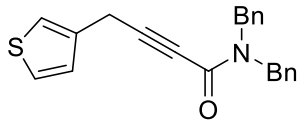


mx5c-178A-PFinal

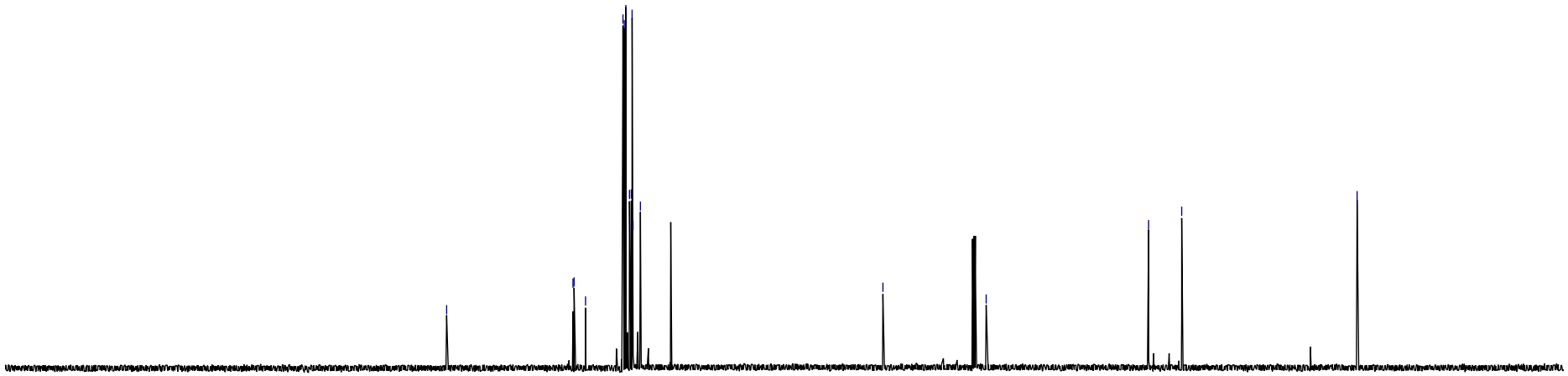
Std carbon

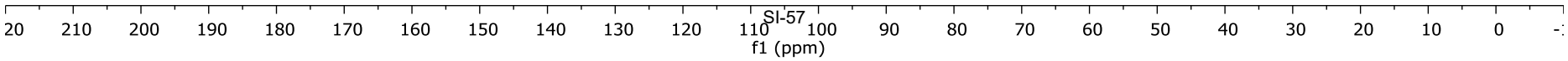
Parameters	
Parameter	Value
Title	mx5c-178A-PFinal
Solvent	cdcl3
Spectrometer Frequency	150.79
Nucleus	13C

154.88
136.23
136.07
134.38
128.86
128.67
128.43
127.89
127.63
127.51
127.36
126.28
90.49
75.24
51.28
46.38
20.49



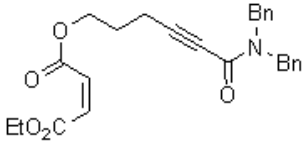
1o





xg-2-227B-h

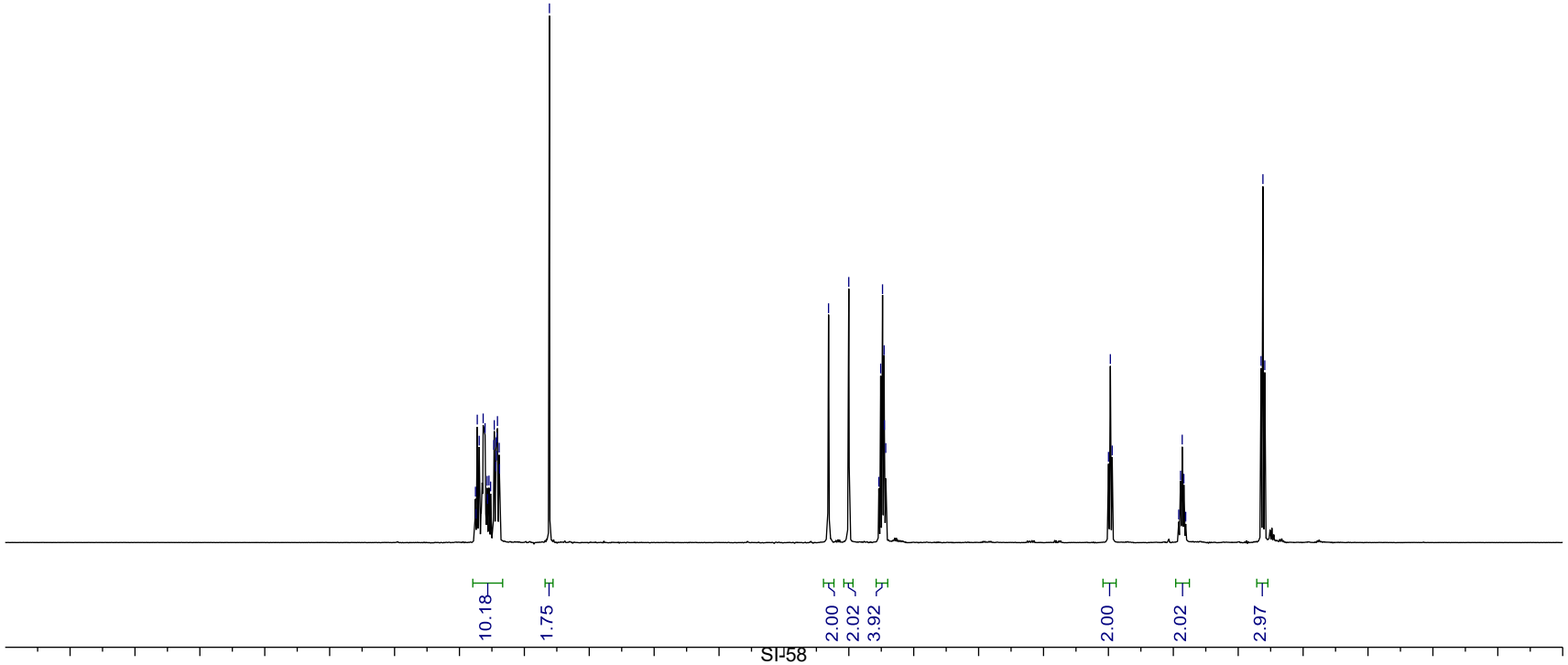
Parameter	Value
1 Title	xg-2-227B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



7.37 7.36 7.35 7.32 7.30 7.29 7.28 7.27 7.26 7.24 7.23 7.22 7.22 7.22 7.21 7.21 7.19 7.19 6.81

4.66 4.50 4.27 4.25 4.24 4.23 4.23 4.22

2.50 2.49 2.47 1.96 1.94 1.93 1.92 1.90 1.32 1.31 1.30



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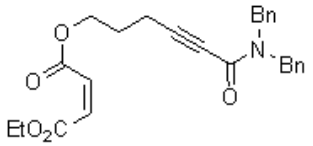
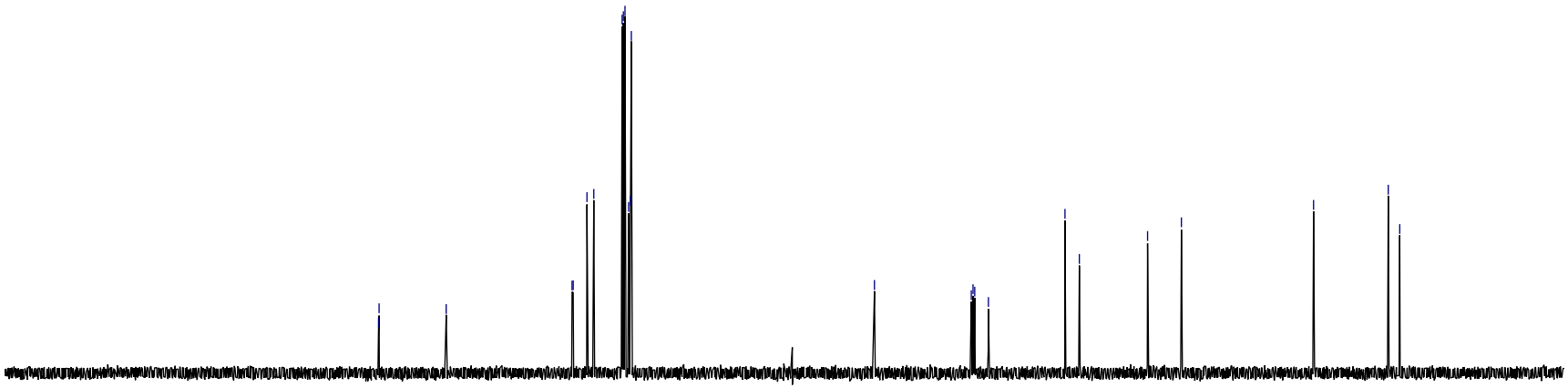
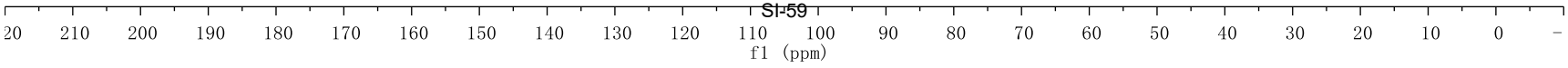
xg-2-227B-c13

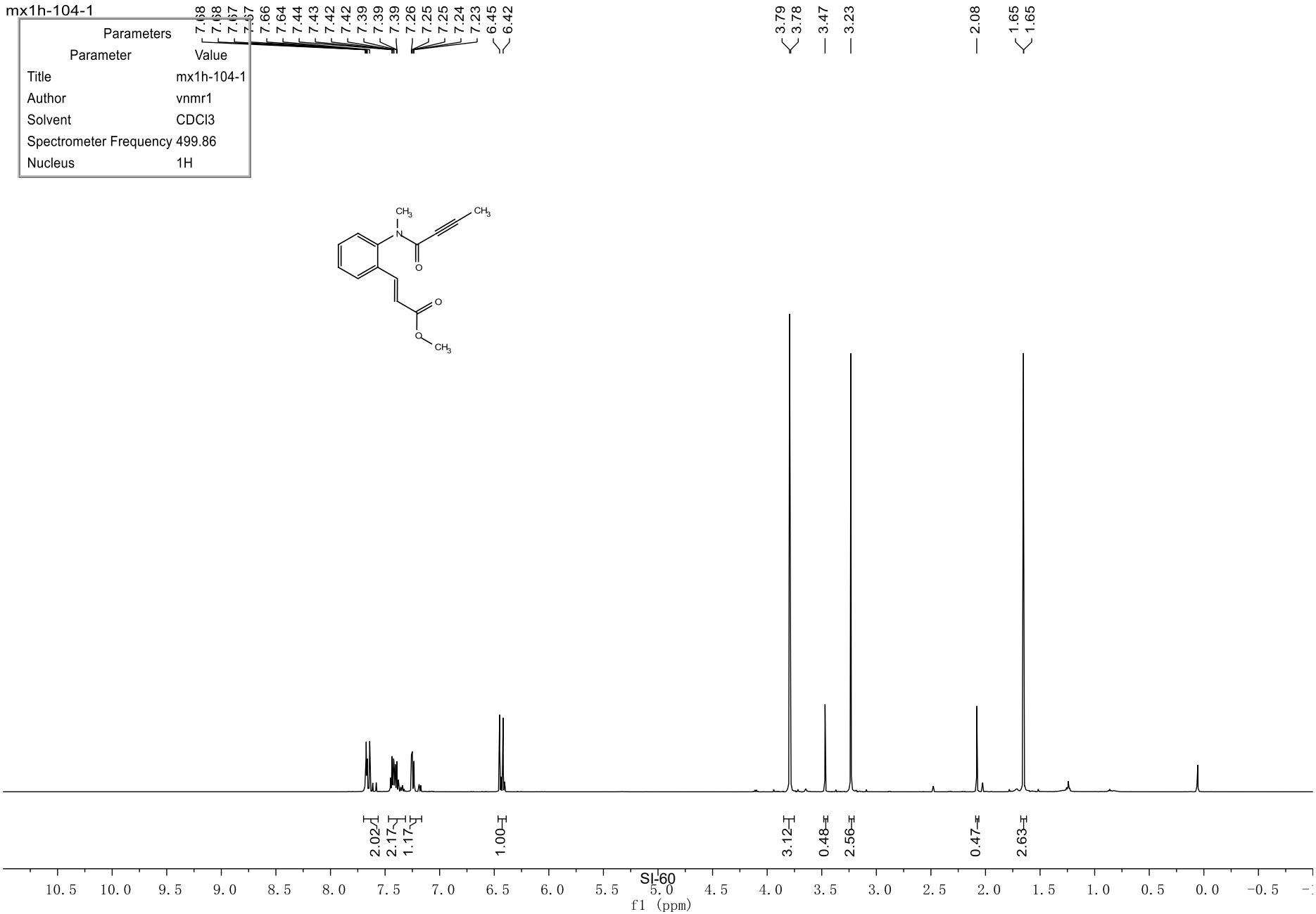
Parameter	Value
1 Title	xg-2-227B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



164.88
164.80
154.89
136.32
136.15
134.12
133.11
128.93
128.75
128.51
127.98
127.70
127.58
91.70
77.41
77.16
76.90
74.88
63.59
61.47
51.40
46.41
26.91
15.88
14.19



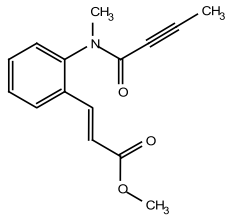


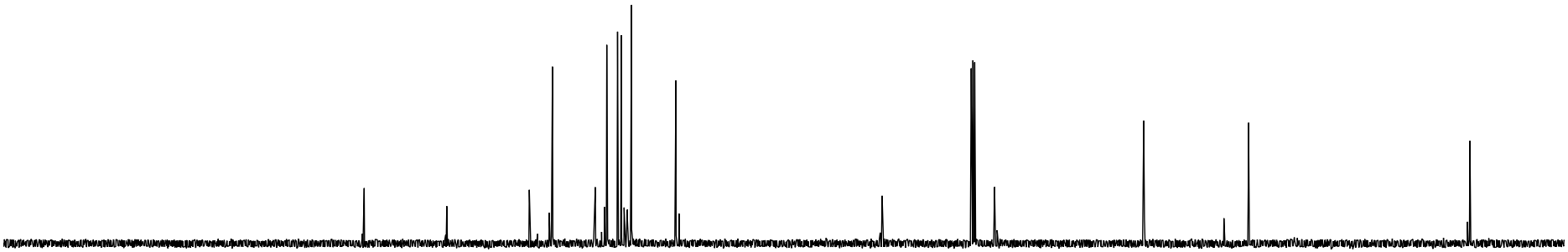

mx1h-104-1
Parameters
Parameter Value
Title mx1h-104-1
Author vnmr1
Solvent CDCl3
Spectrometer Frequency 499.86
Nucleus 1H
7.68
7.68
7.67
7.67
7.66
7.64
7.44
7.43
7.42
7.42
7.39
7.39
7.39
7.26
7.25
7.25
7.24
7.23
6.45
6.42
3.79
3.78
3.47
3.23
2.08
1.65
1.65
CH3
N
CH3
O
O
O
CH3
2.02
2.17
1.17
1.00
3.12
0.48
2.56
0.47
2.63
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

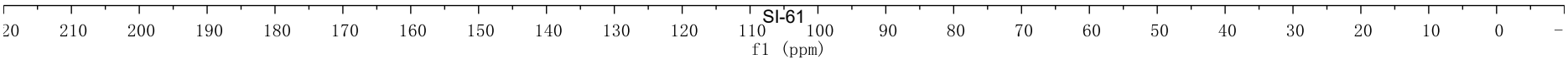
mx1c-104-1

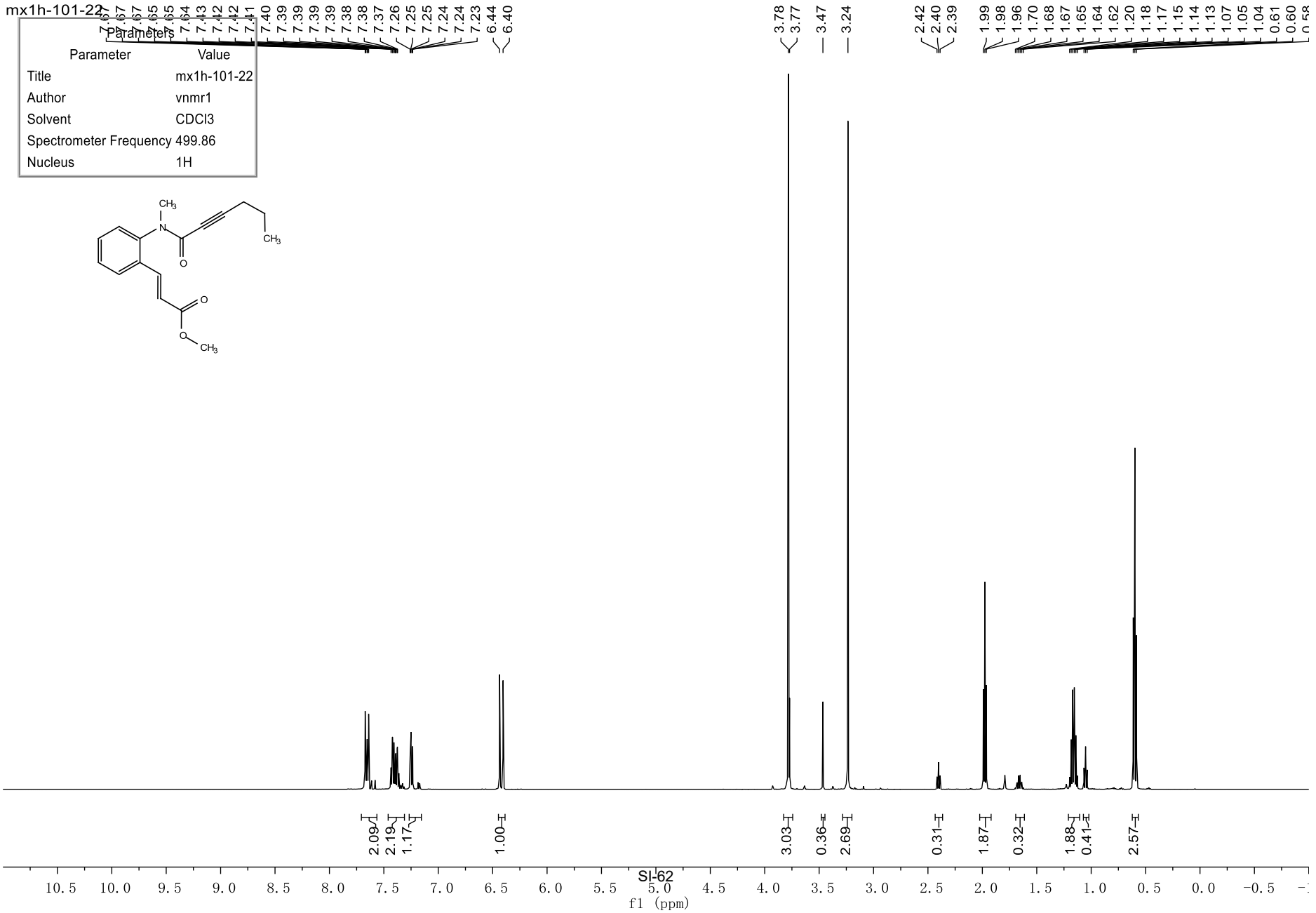
Parameters	
Parameter	Value
Title	mx1c-104-1
Author	
Solvent	CDCl3
Spectrometer Frequency	125.70
Nucleus	13C

166.86
154.69
142.53
139.11
132.81
131.12
129.53
128.98
127.46
120.92
90.54
77.41
77.16
76.91
73.98
51.99
36.54
3.93



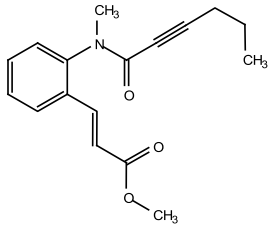




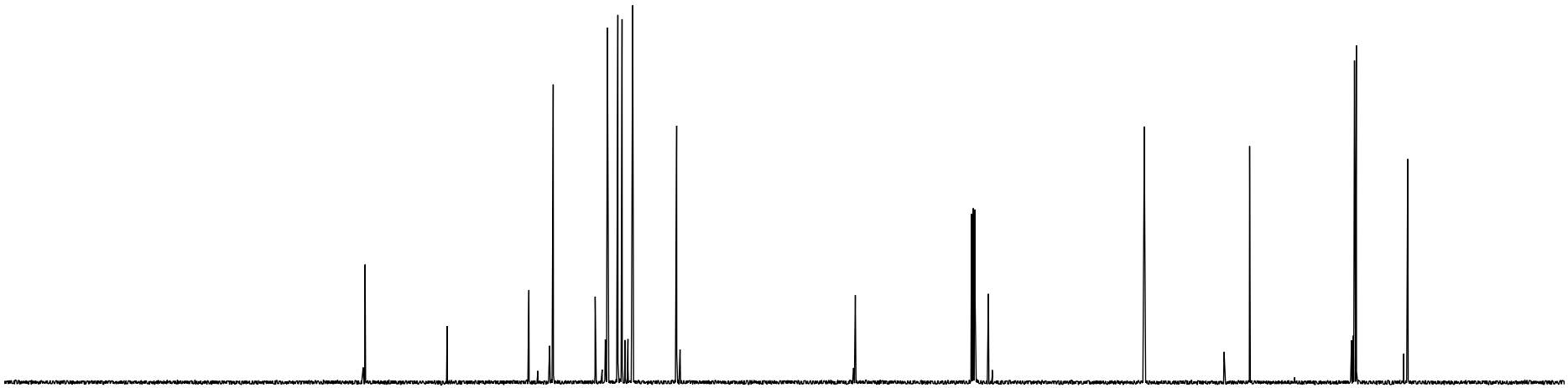

mx1h-101-22
Parameters
Parameter Value
Title mx1h-101-22
Author vnmr1
Solvent CDCl3
Spectrometer Frequency 499.86
Nucleus 1H
7.67 7.67 7.67 7.65 7.65 7.64 7.43 7.42 7.42 7.41 7.40 7.39 7.39 7.39 7.39 7.38 7.38 7.37 7.26 7.25 7.25 7.24 7.24 7.23 6.44 6.40
3.78 3.77 3.47 3.24
2.42 2.40 2.39
1.99 1.98 1.96 1.70 1.68 1.67 1.65 1.64 1.62 1.20 1.18 1.17 1.15 1.14 1.13 1.07 1.05 1.04 0.61 0.60
2.09 2.19 1.17 1.00 3.03 0.36 2.69 0.31 1.87 0.32 1.88 0.41 2.57
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

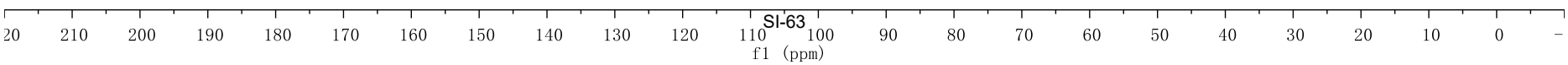
mx1c-101-23

Parameters	
Parameter	Value
Title	mx1c-101-23
Author	
Solvent	CDCl3
Spectrometer Frequency	125.70
Nucleus	13C



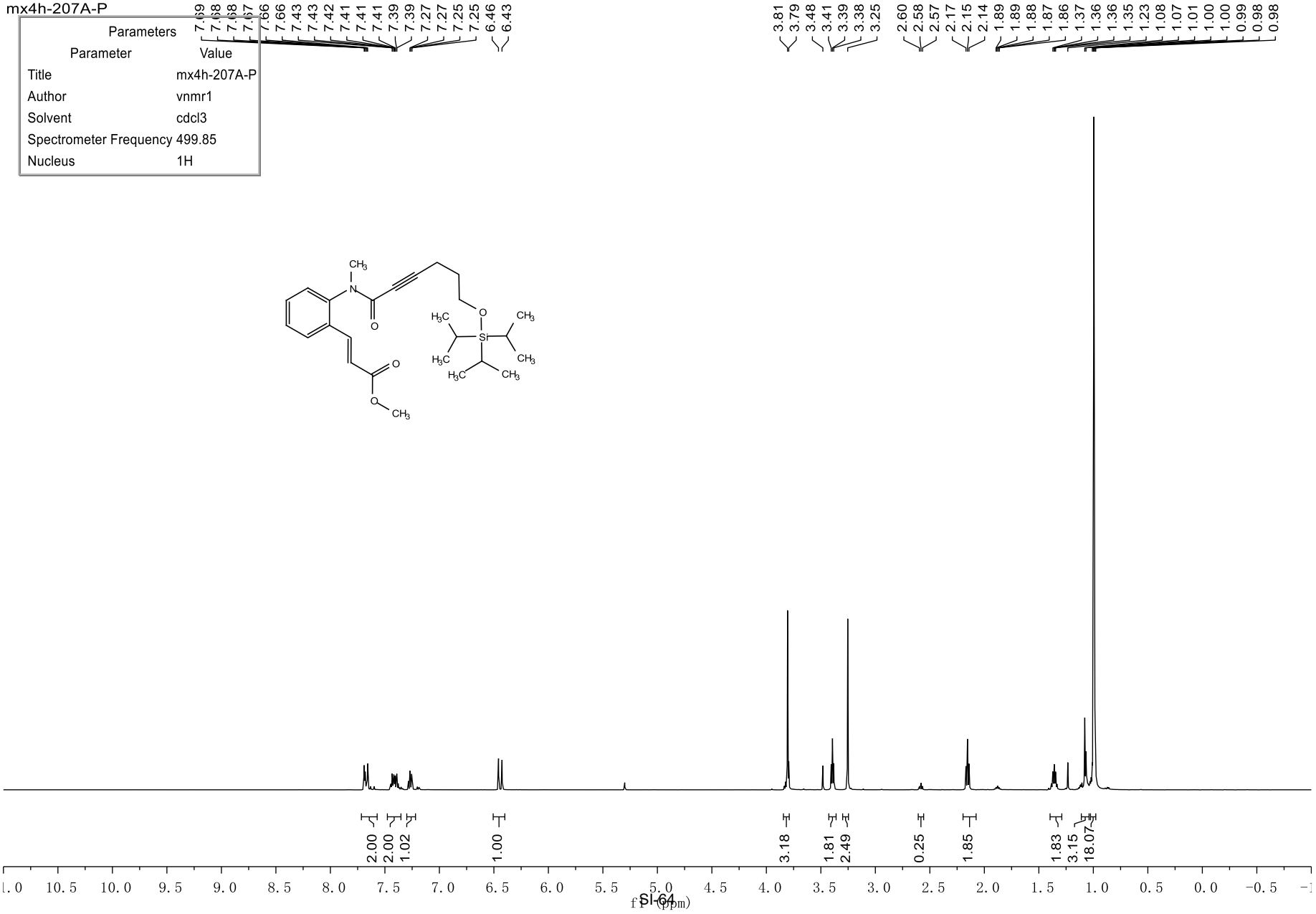
166.81
154.72
142.67
139.08
132.90
131.10
129.55
128.93
127.37
120.89
94.55
77.42
77.16
76.91
74.93
51.95
51.95
36.42
20.96
20.68
13.11





mx4h-207A-P

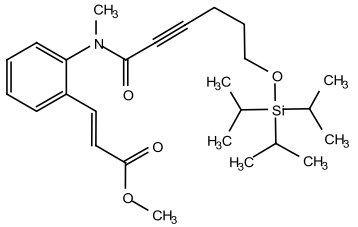
Parameters	
Parameter	Value
Title	mx4h-207A-P
Author	vnmr1
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H



mx4c-207A-P

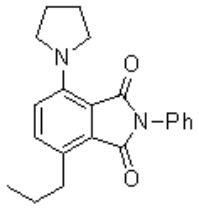
Parameters	
Parameter	Value
Title	mx4c-207A-P
Author	
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

166.75
154.63
142.67
139.01
132.84
131.03
129.59
128.92
127.32
120.89
94.58
77.41
77.16
76.91
74.68
61.26
51.94
36.42
31.00
18.10
18.03
18.02
15.17
11.96



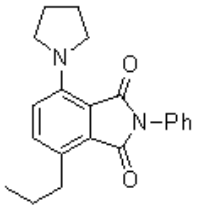
xg-2-222A-h

Parameter	Value
1 Title	xg-2-222A-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

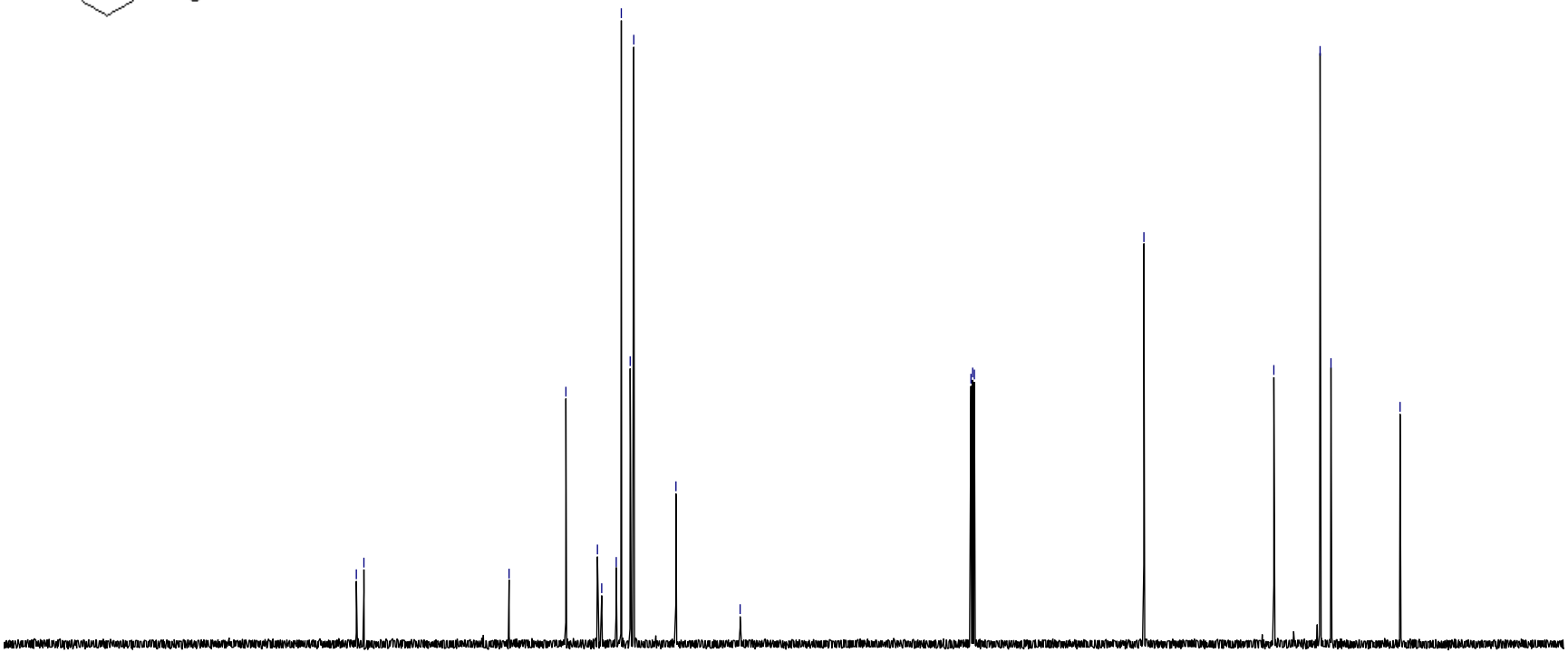


xg-2-222A-c13-2

Parameter	Value
1 Title	xg-2-222A-c13-2
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C

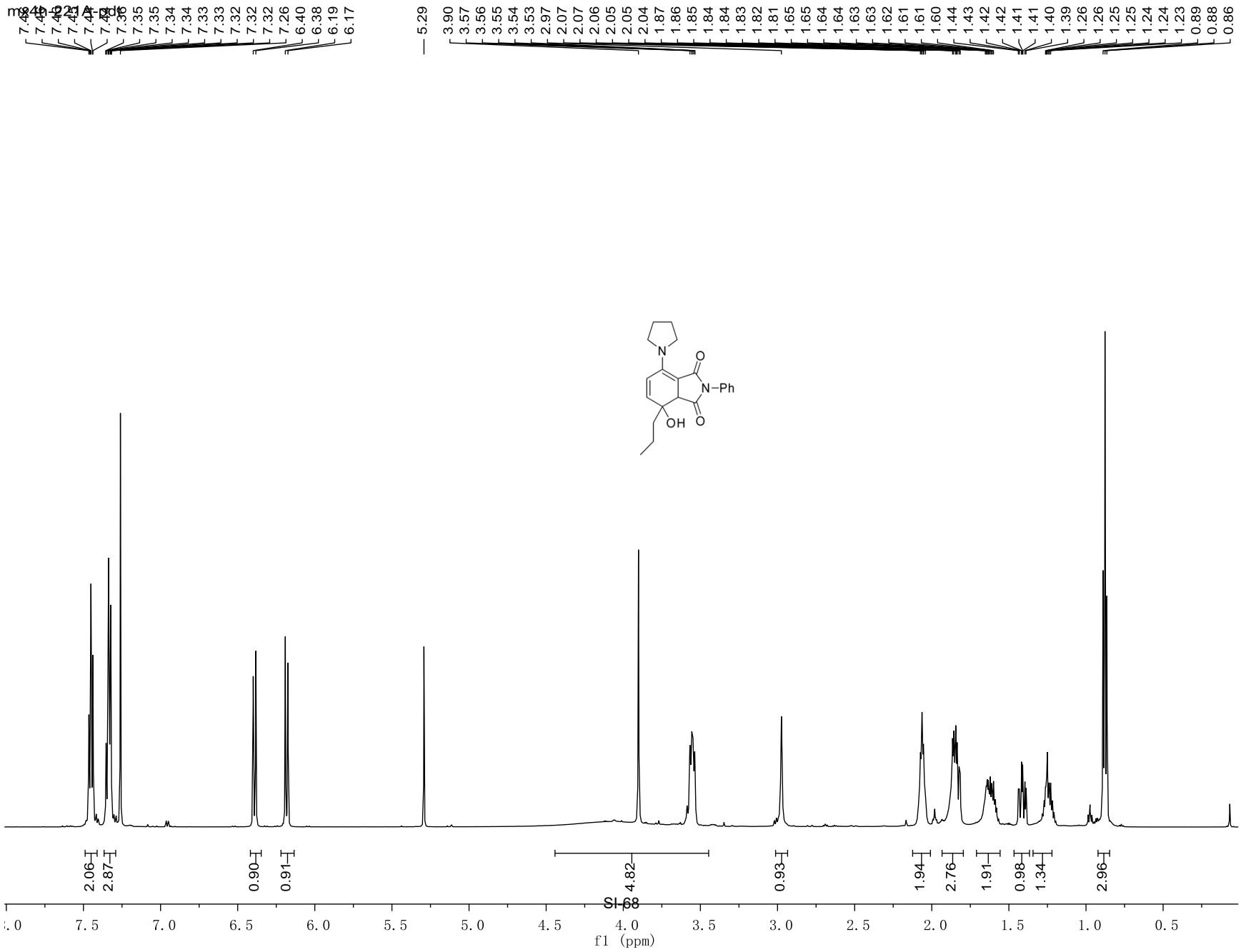


168.04
166.93
145.52
137.14
132.49
131.86
129.72
128.97
127.66
127.13
120.91
111.45
77.42
77.16
76.91
51.91
32.75
25.93
24.33
14.14



220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

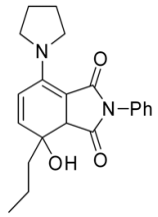
f1 (ppm)

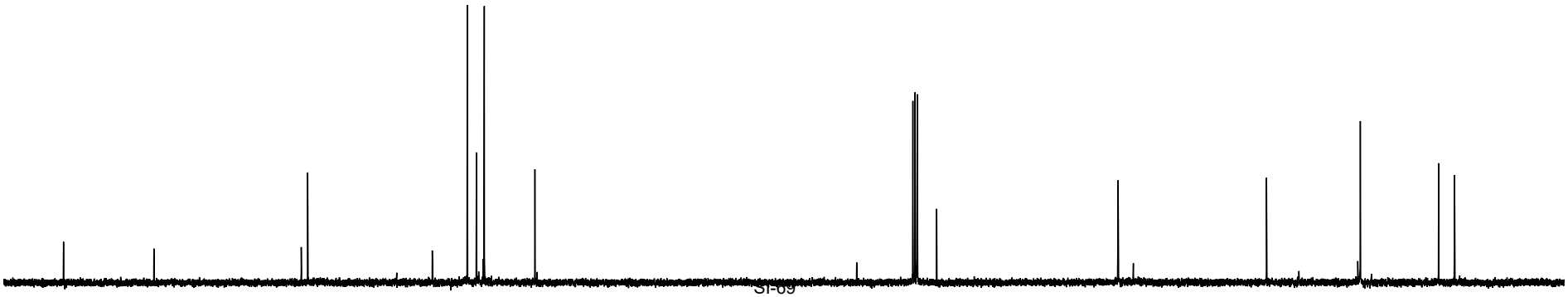

ms4b-221A-pdb
7.48
7.48
7.47
7.47
7.46
7.46
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.32
7.26
6.40
6.38
6.19
6.17
5.29
3.90
3.57
3.56
3.55
3.54
3.53
2.97
2.07
2.06
2.05
2.05
2.04
1.87
1.86
1.85
1.84
1.84
1.83
1.82
1.81
1.65
1.65
1.64
1.64
1.63
1.63
1.62
1.61
1.61
1.60
1.44
1.43
1.42
1.42
1.41
1.41
1.40
1.39
1.26
1.26
1.25
1.25
1.24
1.24
1.23
0.89
0.88
0.86
N
O
N–Ph
O
OH
2.06
2.87
0.90
0.91
4.82
0.93
1.94
2.76
1.91
0.98
1.34
2.96
SI-68
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

mx4c-248A-Pbottom

Parameter	Value
Title	mx4c-248A-Pbottom
Author	
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

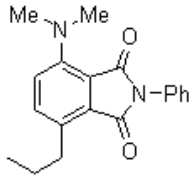
175.
165.
148.20
147.45
133.04
128.98
128.97
127.93
127.13
127.01
121.16
83.92
77.41
77.16
76.91
74.66
53.66
51.90
36.49
25.93
25.63
16.57
14.73





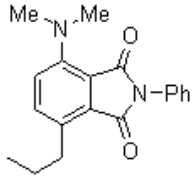
xg-2-213B-h

Parameter	Value
1 Title	xg-2-213B-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

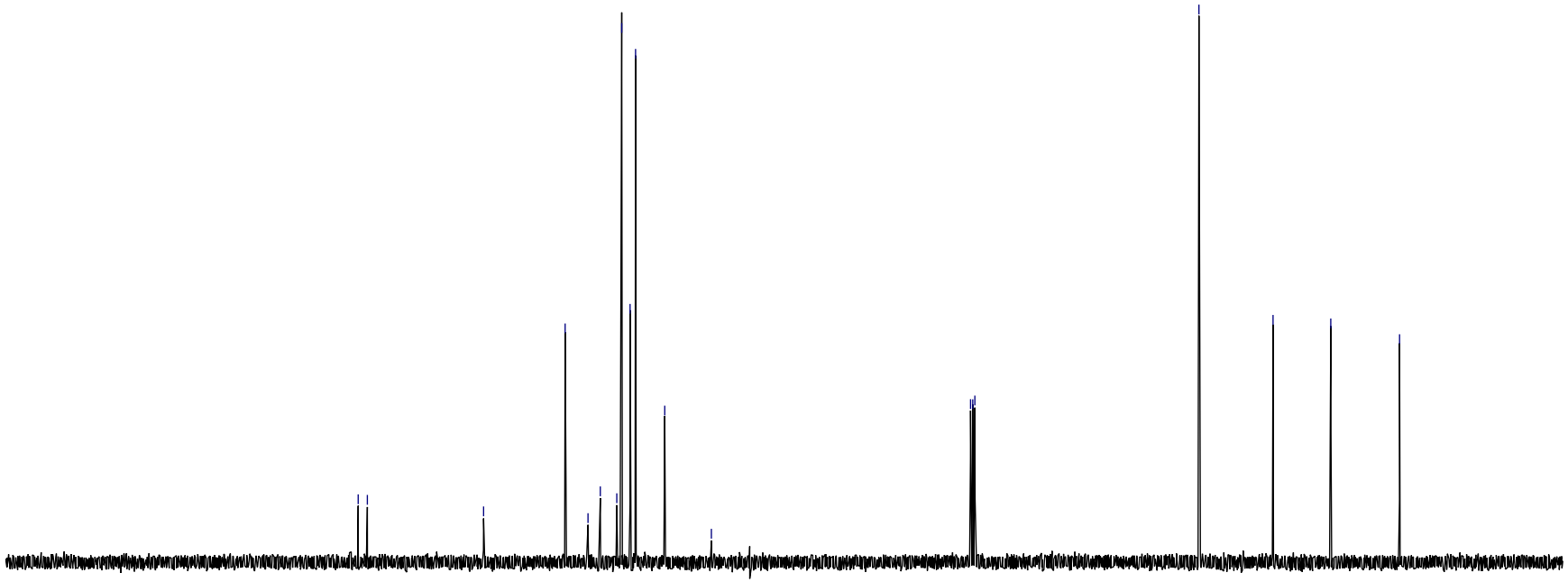


xg-2-213B-c13

Parameter	Value
1 Title	xg-2-213B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



167.92
166.57
149.40
137.36
133.98
132.16
129.73
129.00
127.76
126.95
122.65
115.76
77.48
77.15
76.84
43.75
32.80
24.27
14.11

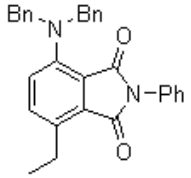


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 –

f1 (ppm)

xg-2-222B-h

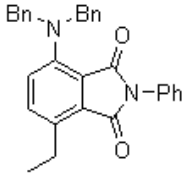
Parameter	Value
1 Title	xg-2-222B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



xg-2-222B-c13

Parameter	Value
1 Title	xg-2-222B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C

167.33
166.60
148.11
137.90
136.66
136.42
132.17
129.70
129.05
128.56
128.17
127.87
127.32
127.07
126.15
118.21
77.41
77.16
76.91
56.61
24.11
14.99

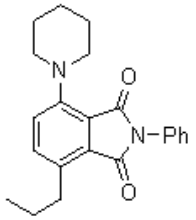


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 –

f1 (ppm)

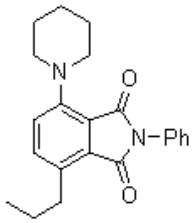
xg-2-213CC-h

Parameter	Value
1 Title	xg-2-213CC-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

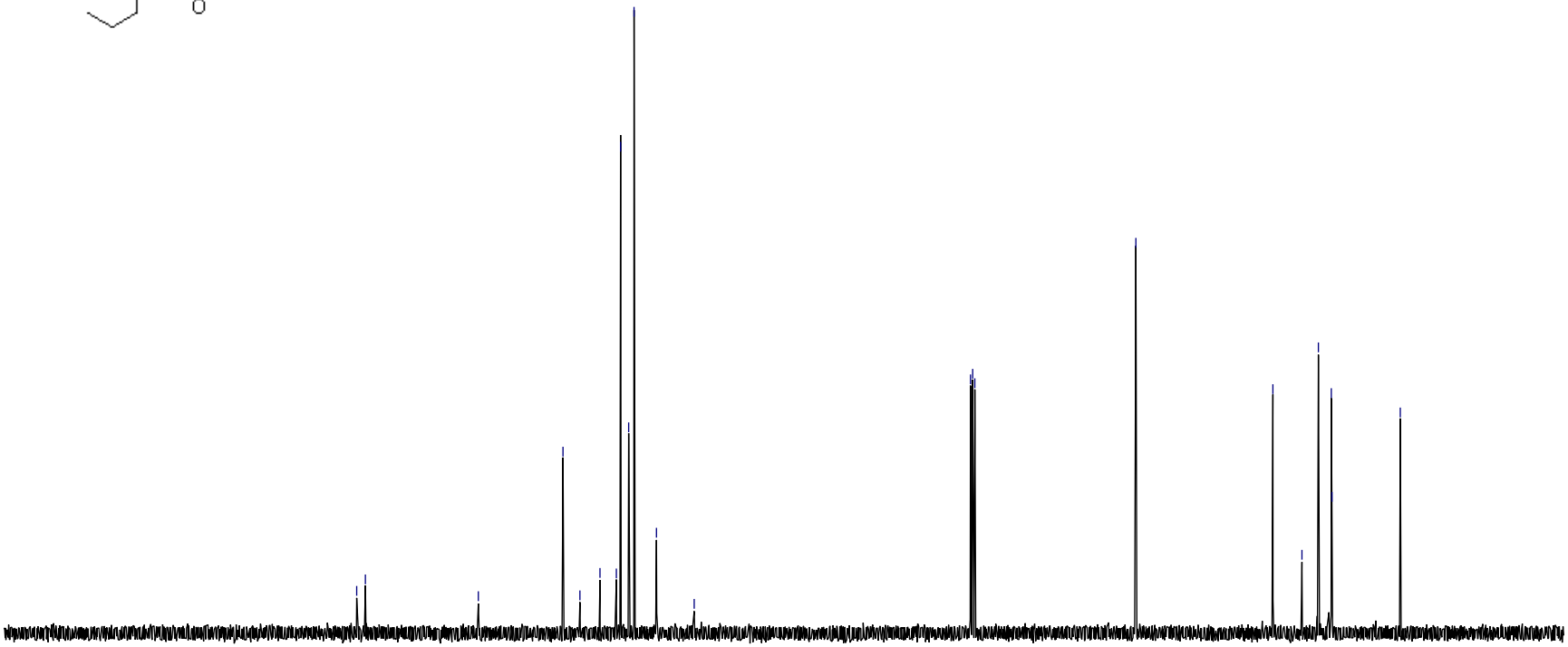


xg-2-213CC-c13

Parameter	Value
1 Title	xg-2-213CC-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



167.99
166.71
150.05
137.57
135.08
132.12
129.70
129.08
127.89
127.09
123.79
118.22
77.48
77.16
76.84
53.10
32.89
28.61
26.18
24.28
24.18
14.11

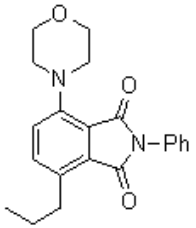


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

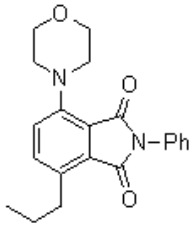
xg-2-213DD-h

Parameter	Value
1 Title	xg-2-213DD-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

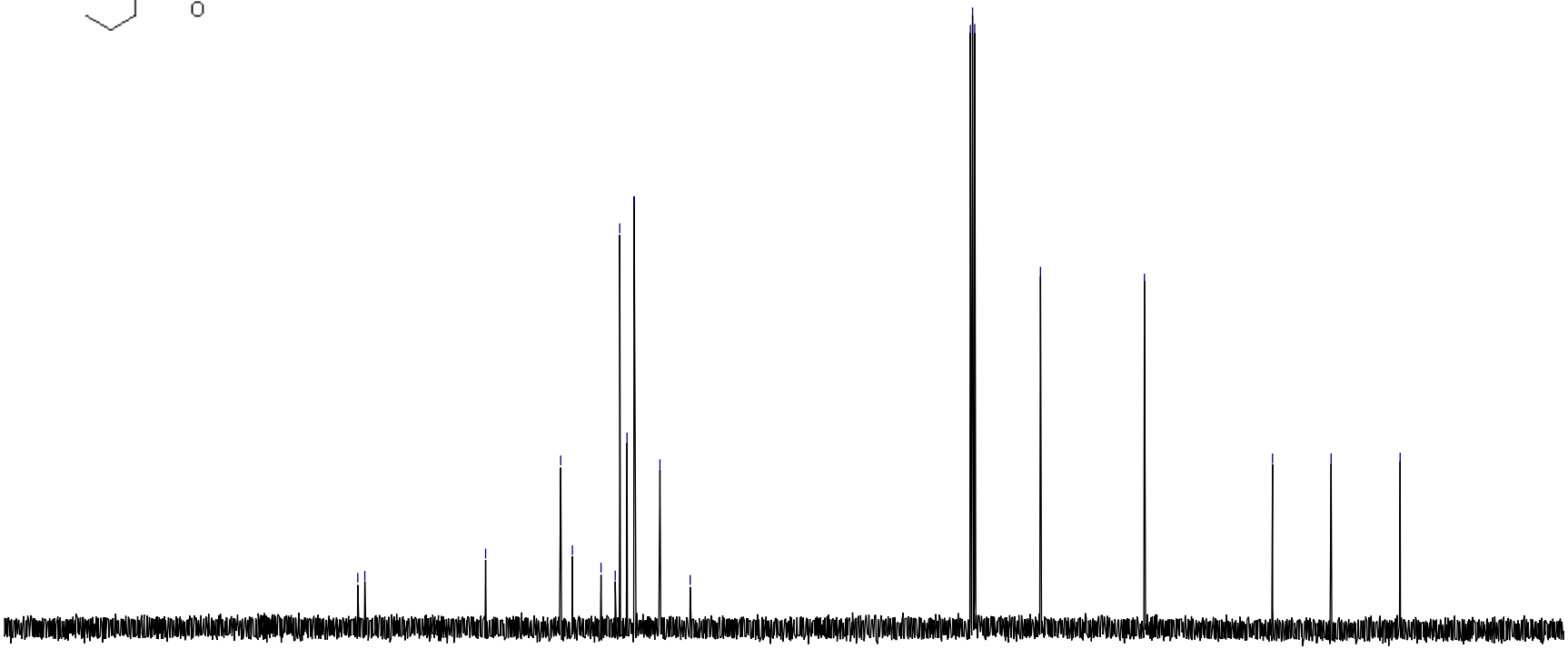


xg-2-213DD-c13

Parameter	Value
1 Title	xg-2-213DD-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



167.81
166.78
148.96
137.89
136.17
131.94
129.85
129.18
128.11
127.07
123.25
118.80
77.48
77.16
76.84
67.14
51.82
32.92
24.28
14.11

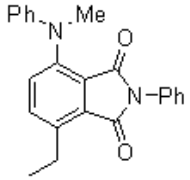


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 –

f1 (ppm)

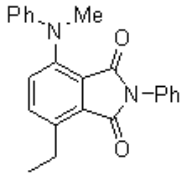
xg-2-202A-h

Parameter	Value
1 Title	xg-2-202A-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

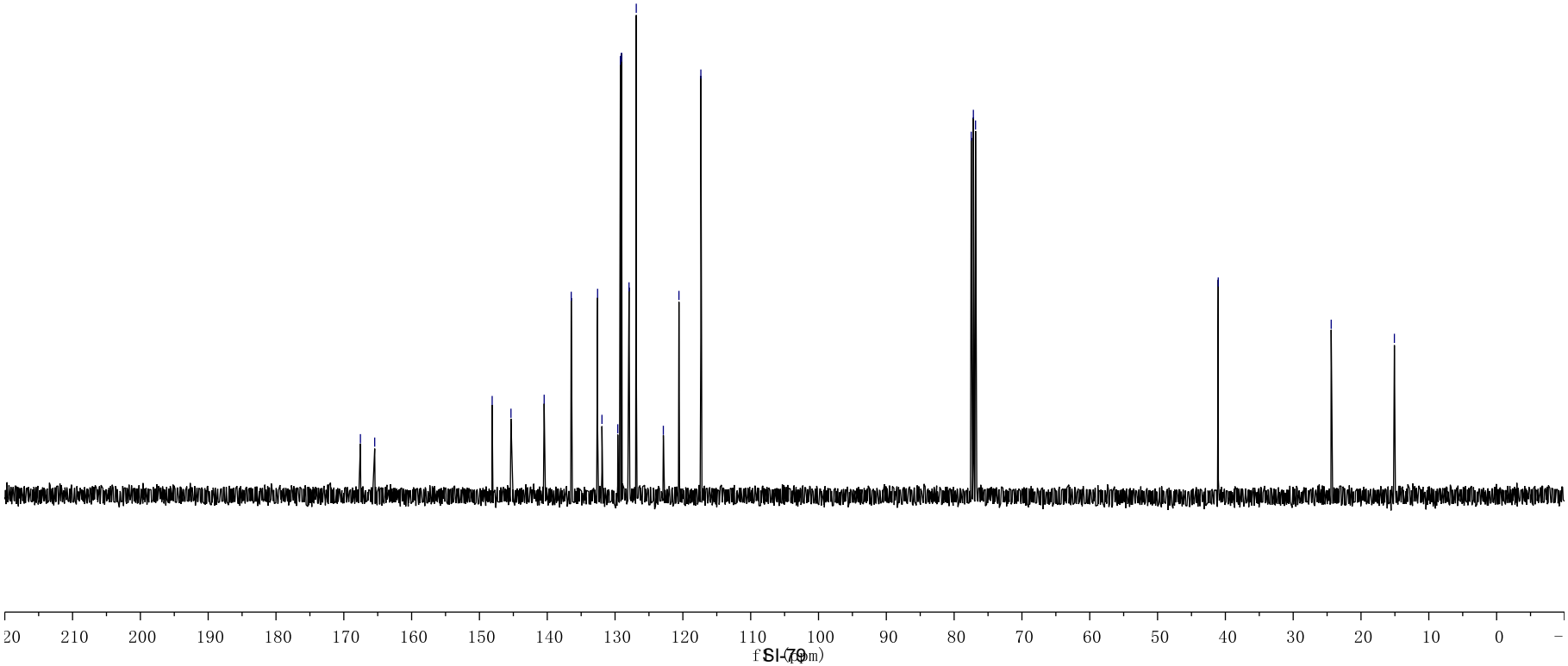


xg-2-202A-c13

Parameter	Value
1 Title	xg-2-202A-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C

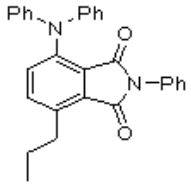


167.55
165.44
148.12
145.35
140.46
136.46
132.58
131.93
129.60
129.21
129.05
127.94
126.87
122.88
120.58
117.35
77.48
77.16
76.84
41.05
24.39
15.08



xg-2-202B-h

Parameter	Value
1 Title	xg-2-202B-h
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H



7.43 7.42 7.41 7.41 7.39 7.33 7.33 7.31 7.31 7.29 7.27 7.26 7.25 7.25 7.09 7.09 7.07 7.06 7.04 7.03 7.02 7.02

3.13 3.12 3.11 3.11 3.09

1.78 1.76 1.76 1.75 1.74 1.72 1.07 1.05 1.03

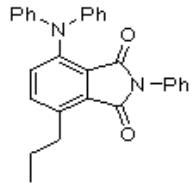
2.98 8.10 5.97 2.00 2.02 3.03

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5

f1 (ppm)

xg-2-202B-c13

Parameter	Value
1 Title	xg-2-202B-c13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C

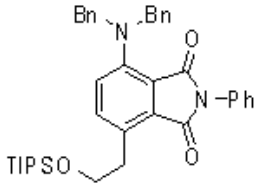


167.47
164.28
147.85
143.37
139.09
137.40
133.52
131.86
129.88
129.31
128.92
127.73
126.78
123.65
123.47
123.45
77.48
77.16
76.84
33.19
24.23
14.21

f1 (ppm)

xg-2-225B-h

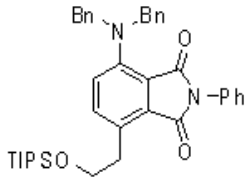
Parameter	Value
1 Title	xg-2-225B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



7.52 7.51 7.49 7.47 7.47 7.46 7.43 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.37 7.37 7.30 7.30 7.30 7.29 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.12 7.10 4.56 4.00 3.99 3.98 3.31 3.30 3.29 1.02 1.01 0.99 0.97

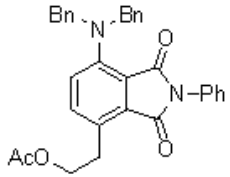
xg-2-225B-c13

Parameter	Value
1 Title	xg-2-225B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



xg-3-36B-h

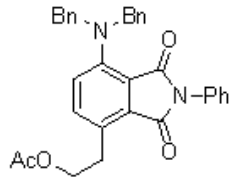
Parameter	Value
1 Title	xg-3-36B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

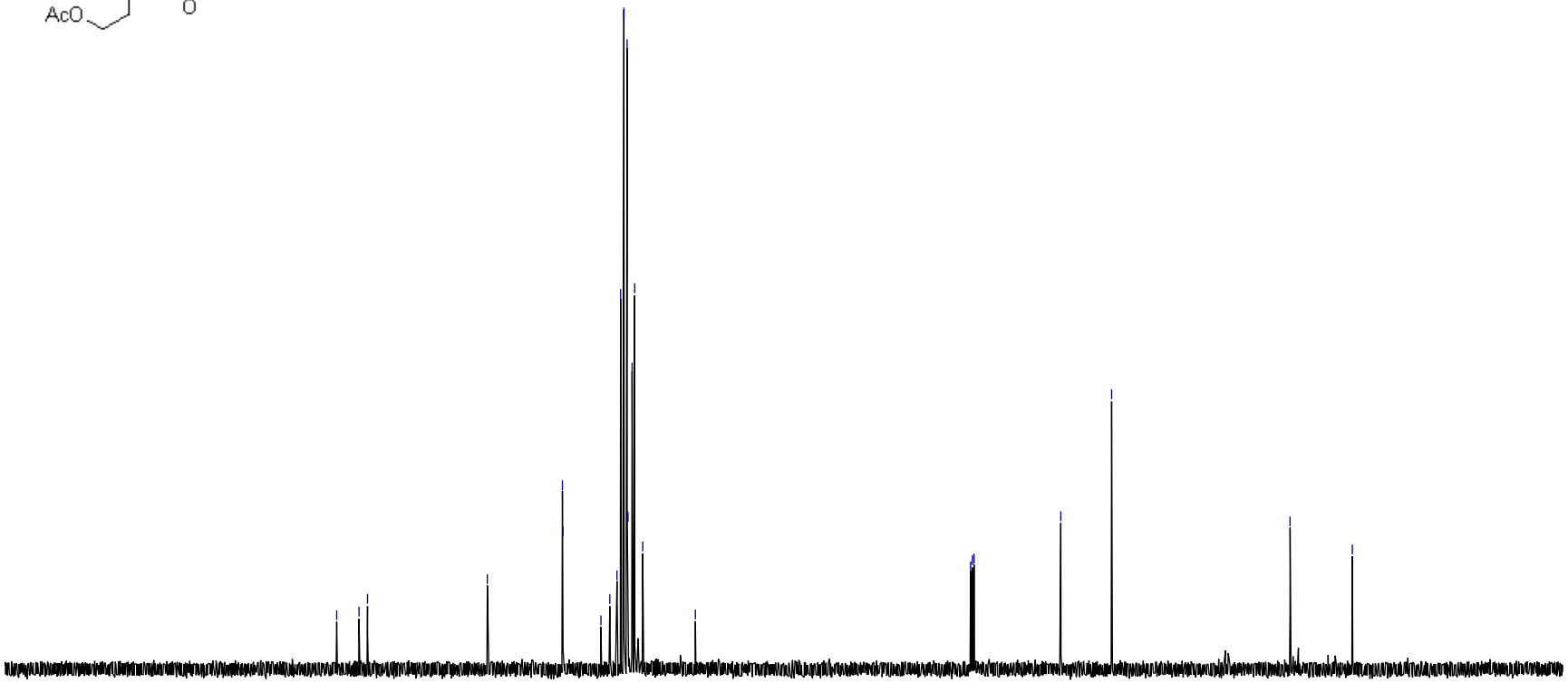


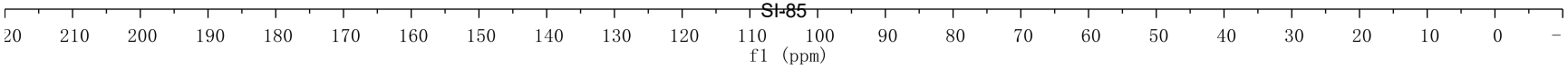
xg-3-36B-c13

Parameter	Value
1 Title	xg-3-36B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C

171.00
167.71
166.45
148.76
137.68
137.61
131.99
130.68
129.62
129.08
128.60
128.12
127.99
127.39
127.01
125.82
118.05
77.41
77.16
76.91
64.10
56.59
30.24
21.05

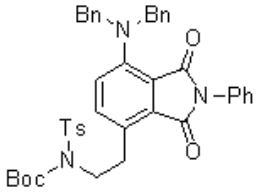






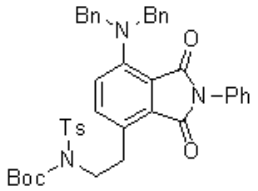
xg-2-243Apure-h

Parameter	Value
1 Title	xg-2-243Apure-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H



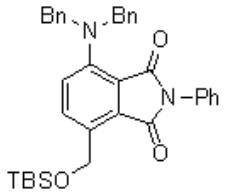
xg-2-243Apure-c13

Parameter	Value
1 Title	xg-2-243Apure-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C



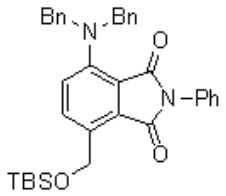
xg-2-241B-h

Parameter	Value
1 Title	xg-2-241B-h
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86
5 Nucleus	1H

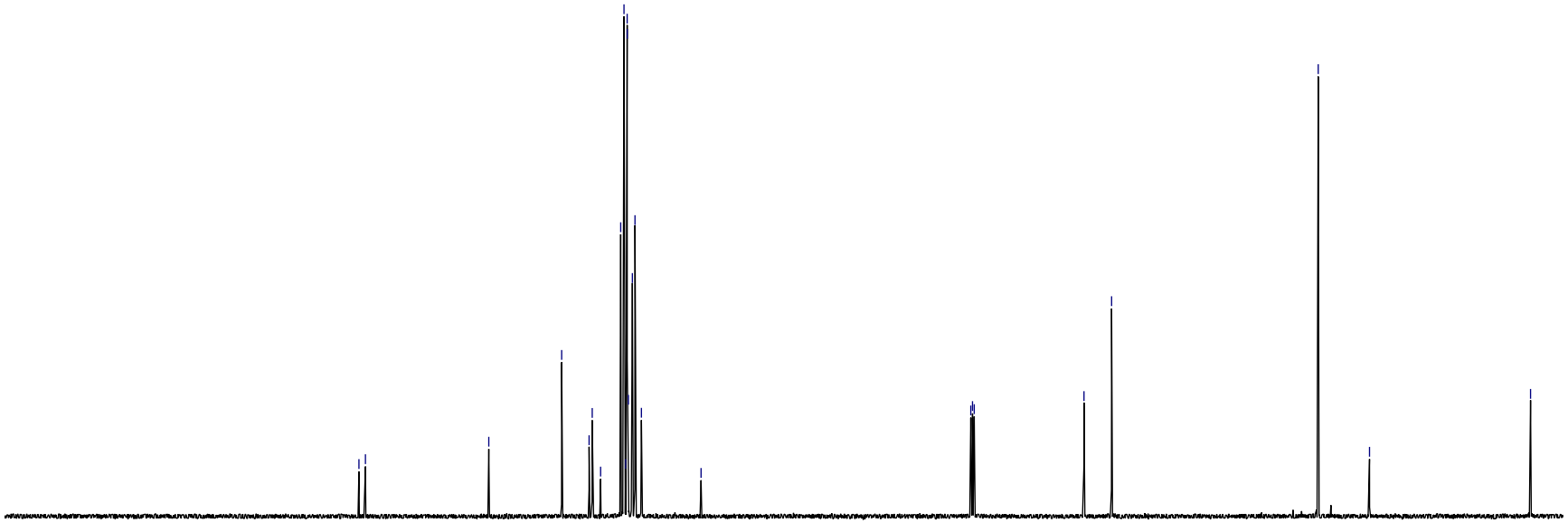


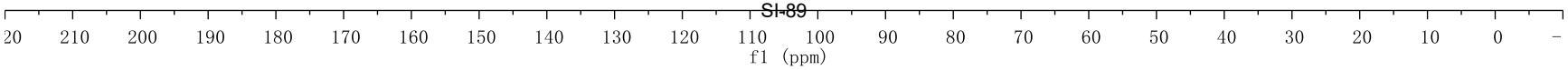
xg-2-241B-c13

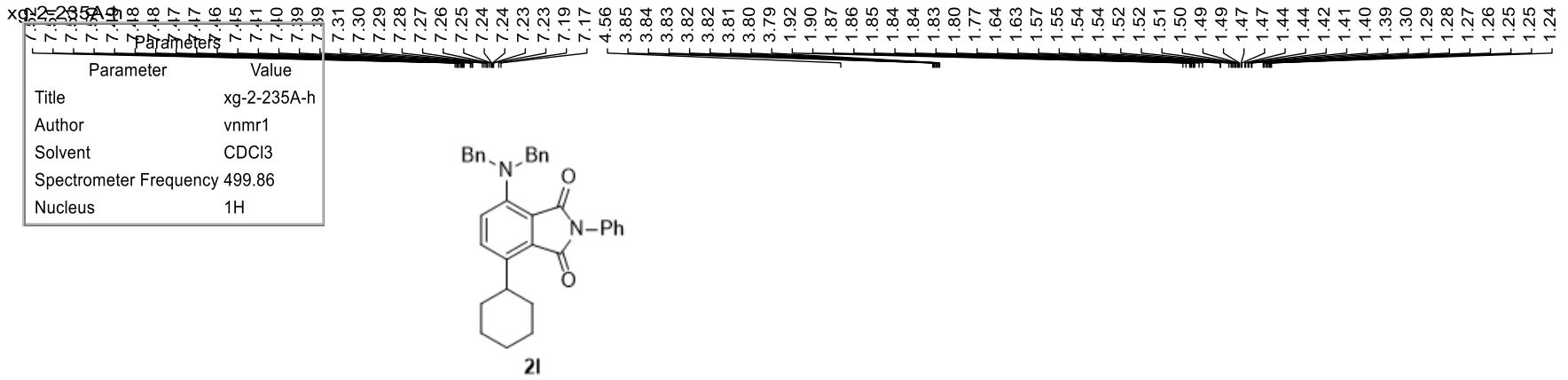
Parameter	Value
1 Title	xg-2-241B-c13
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70
5 Nucleus	13C

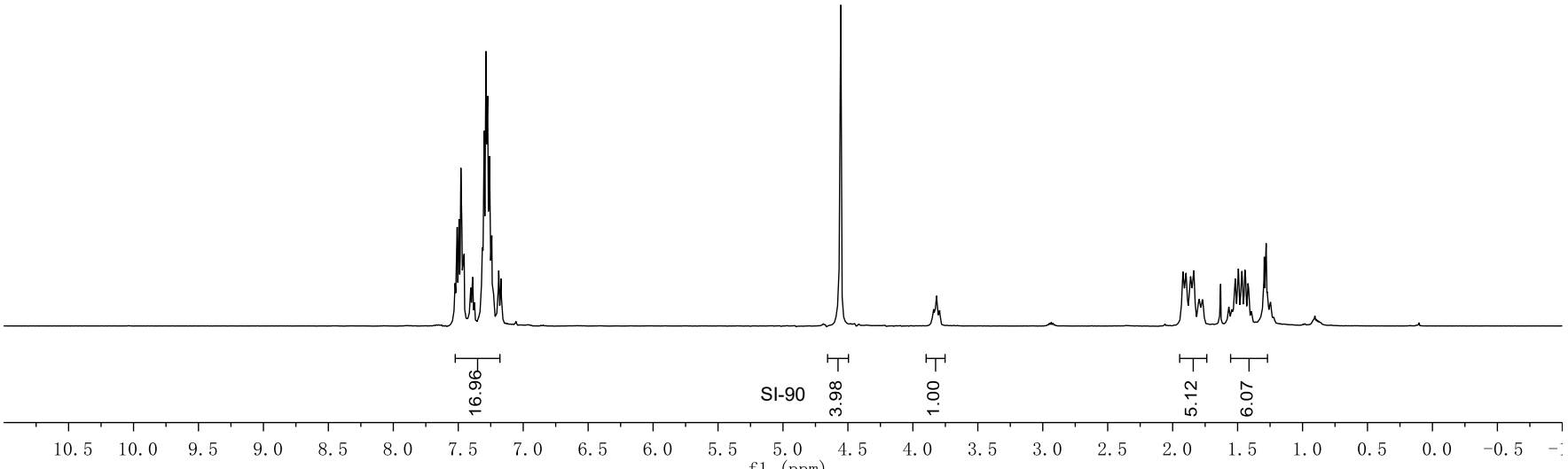


167.74
166.78
148.57
137.81
133.76
133.30
132.06
129.10
128.61
128.38
128.14
128.14
127.96
127.37
126.99
126.04
117.23
77.41
77.16
76.91
60.70
56.63
26.12
18.55
-5.22





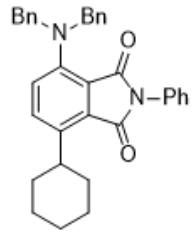

xg-2-235A-h
Parameters
Parameter Value
Title xg-2-235A-h
Author vnmr1
Solvent CDCl3
Spectrometer Frequency 499.86
Nucleus 1H
Bn
N
Bn
O
N–Ph
O
2l


16.96
SI-90
3.98
1.00
5.12
6.07
f1 (ppm)

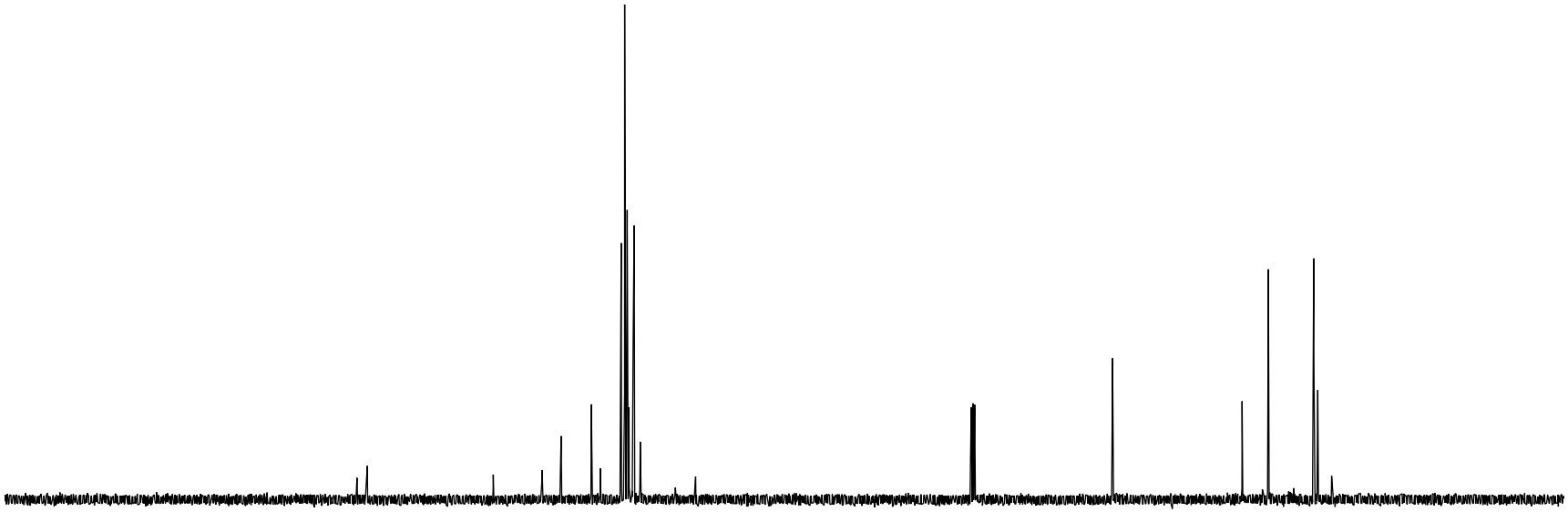
xg-2-235A-c13-

Parameters	
Parameter	Value
Title	xg-2-235A-c13-
Author	
Solvent	CDCl3
Spectrometer Frequency	125.70
Nucleus	13C

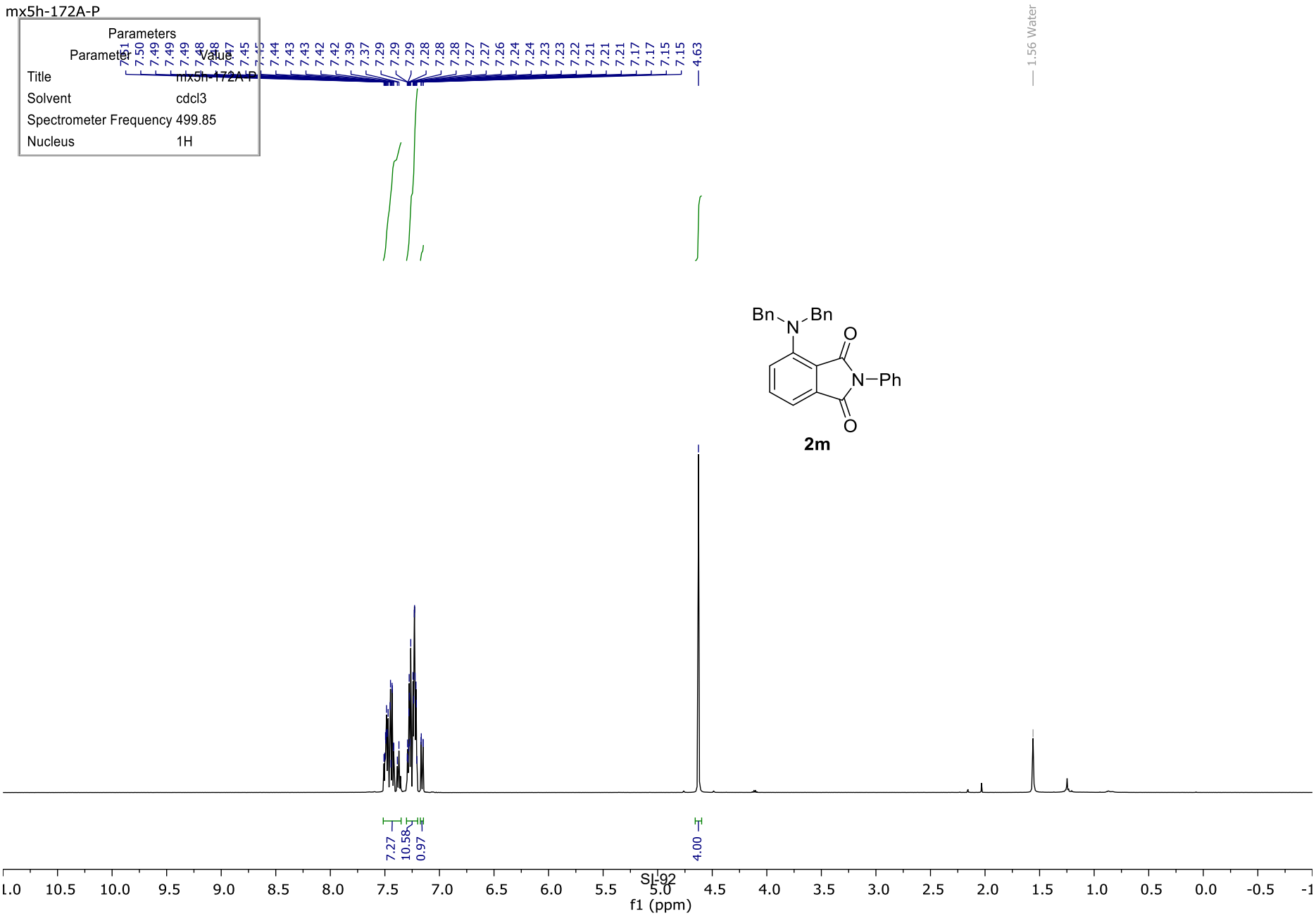
168.06
166.54
147.95
140.74
137.94
133.48
132.16
129.07
129.05
128.56
128.19
127.92
127.31
127.16
126.26
121.08
118.09
56.57
37.45
33.58
26.88
26.36
26.29
24.24



2l



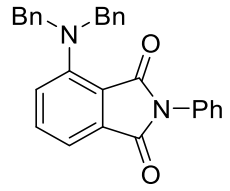
f1 (ppm)


mx5h-172A-P
Parameters
Parameter Value
Title mx5h-172A-P
Solvent cdcl3
Spectrometer Frequency 499.85
Nucleus 1H
7.51 7.50 7.49 7.49 7.49 7.48 7.48 7.47 7.45 7.44 7.43 7.43 7.42 7.42 7.39 7.37 7.29 7.29 7.29 7.28 7.28 7.28 7.27 7.27 7.26 7.24 7.24 7.23 7.23 7.22 7.21 7.21 7.21 7.17 7.17 7.15 7.15 4.63
1.56 Water
Bn N Bn
O
N–Ph
O
2m
7.27
10.58
0.97
4.00
f1 (ppm)

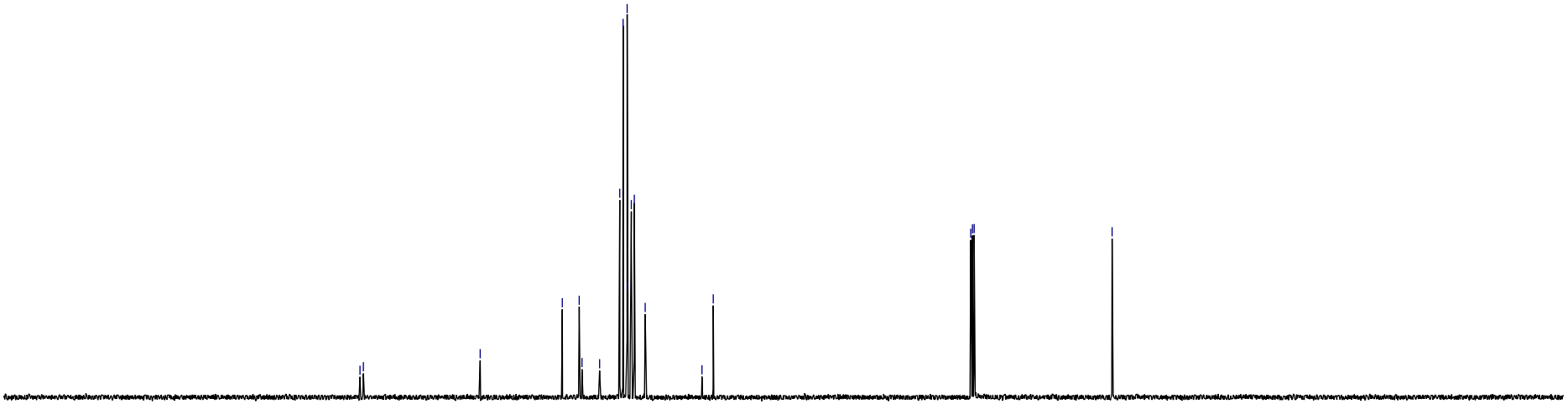
mx5c-172A-P
Std carbon

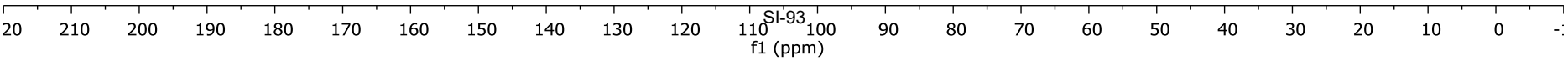
Parameters	
Parameter	Value
Title	mx5c-172A-P
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

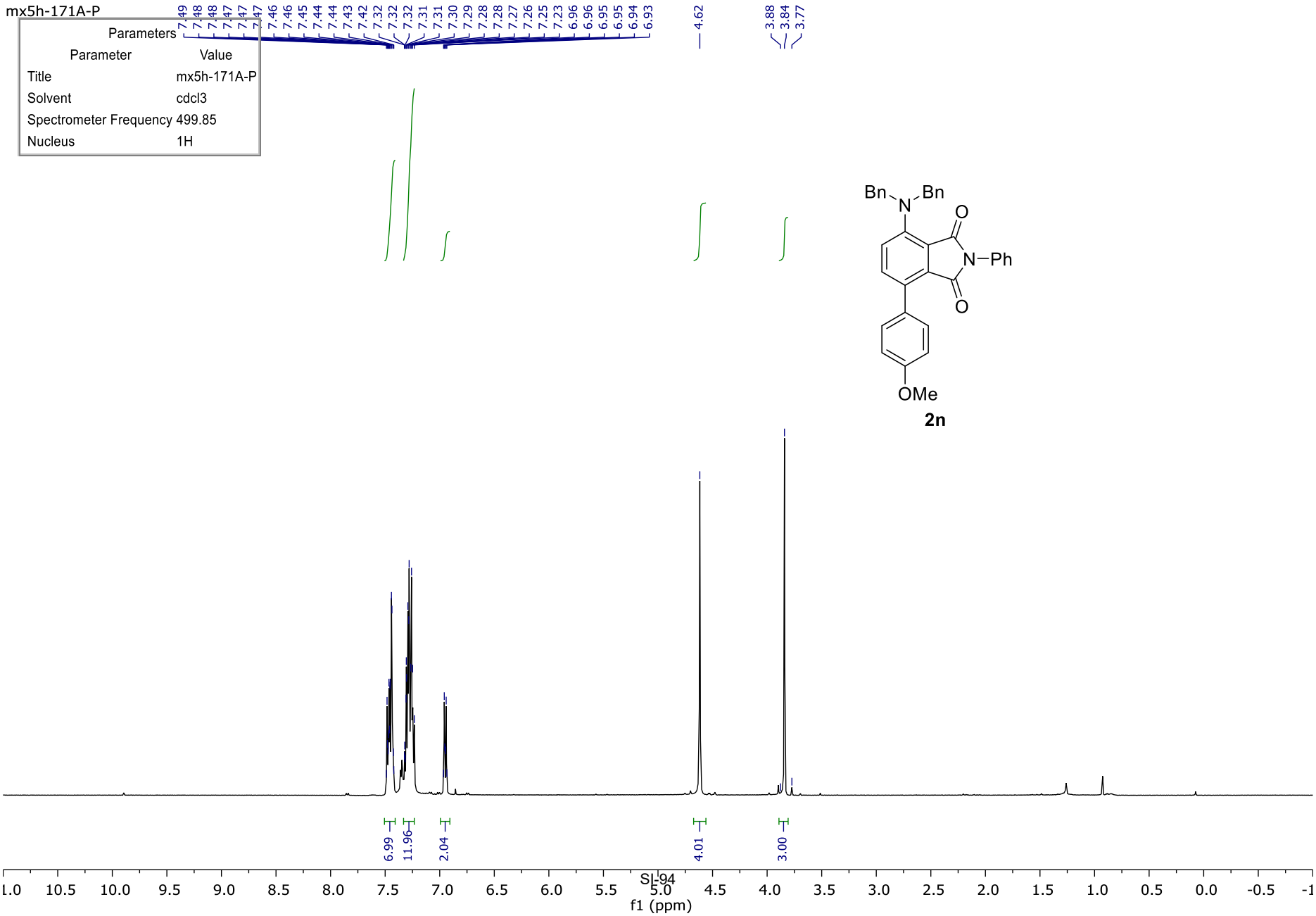
167.45
166.95
149.73
137.63
135.13
134.73
132.13
129.16
128.66
128.07
128.04
127.45
127.01
125.41
117.04
115.37
77.41
77.16
76.91
56.58



2m



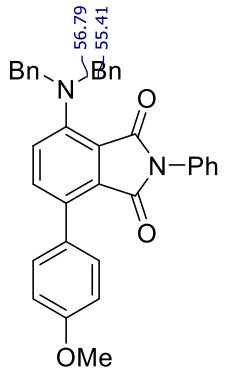



mx5h-171A-P
Parameters
Parameter Value
Title mx5h-171A-P
Solvent cdcl3
Spectrometer Frequency 499.85
Nucleus 1H
7.49 7.48 7.48 7.47 7.47 7.47 7.46 7.46 7.45 7.44 7.44 7.43 7.42 7.32 7.32 7.32 7.31 7.31 7.30 7.29 7.28 7.28 7.27 7.26 7.25 7.23 6.96 6.96 6.95 6.95 6.94 6.93
4.62
3.88 3.84 3.77
Bn N Bn
O
N–Ph
O
OMe
2n
6.99
11.96
2.04
4.01
3.00
f1 (ppm)

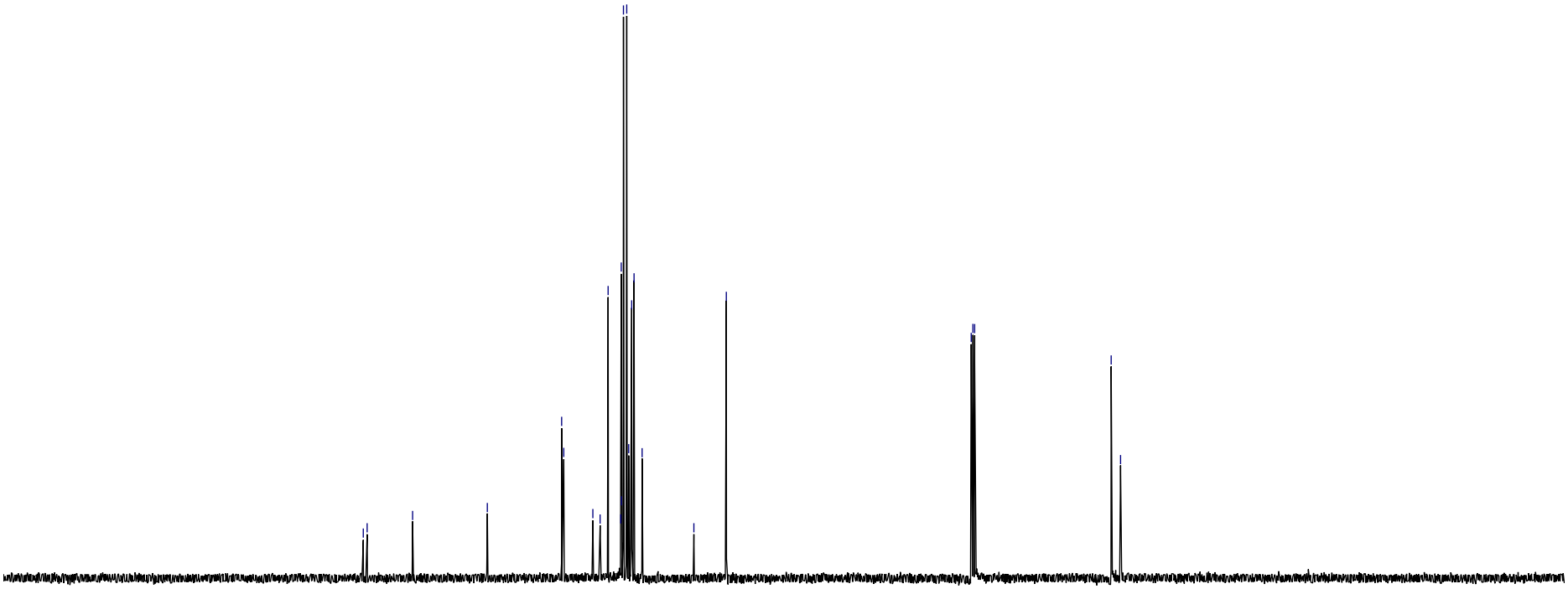
mx5c-171A-Ps3
Std carbon

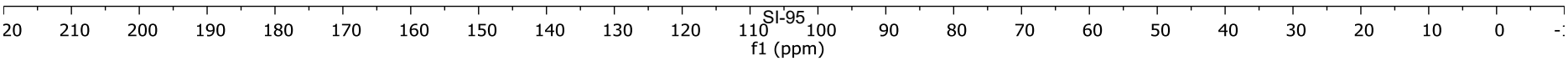
Parameters	
Parameter	Value
Title	mx5c-171A-Ps3
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

166.99
166.42
159.72
148.71
137.76
137.45
133.17
132.10
130.92
129.05
128.98
128.95
128.66
128.17
127.88
127.44
127.10
125.91
118.28
113.50
77.41
77.16
76.90
56.79
55.41



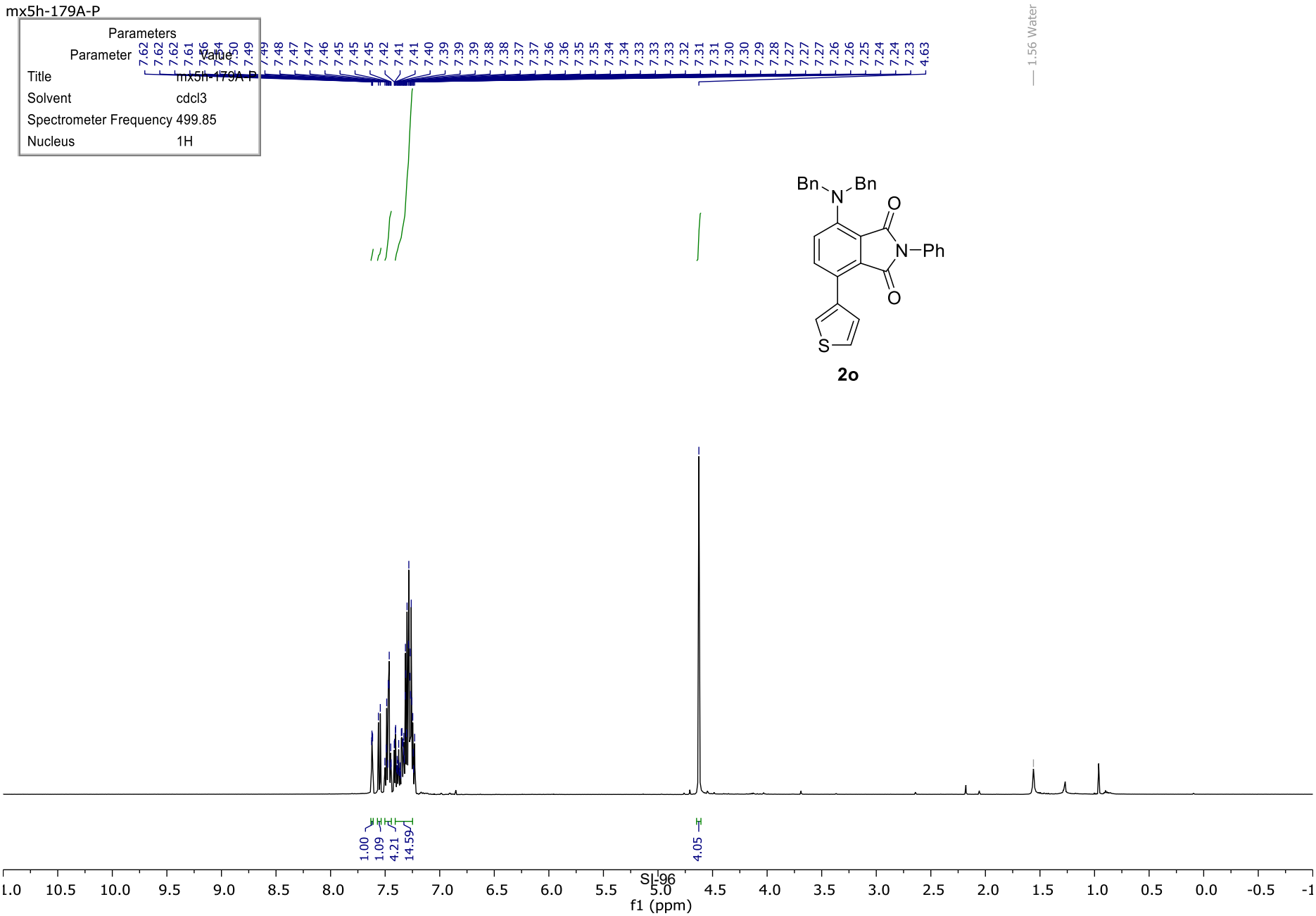
2n





mx5h-179A-P

Parameters	
Parameter	Value
Title	mx5h-179A-P
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H

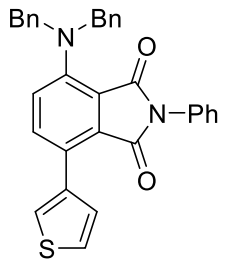


2o

mx5c-179A-P
Std carbon

Parameters	
Parameter	Value
Title	mx5c-179A-P
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

167.02
166.35
148.88
137.67
137.19
137.03
132.06
129.27
129.12
129.06
128.68
128.16
128.00
127.72
127.48
127.12
125.98
124.97
124.66
77.41
77.16
76.91
56.82

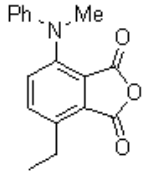


2o

f1 (ppm)

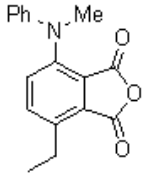
xg-3-69A-

Parameter	Value
1 Title	xg-3-69A-
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78
5 Nucleus	1H

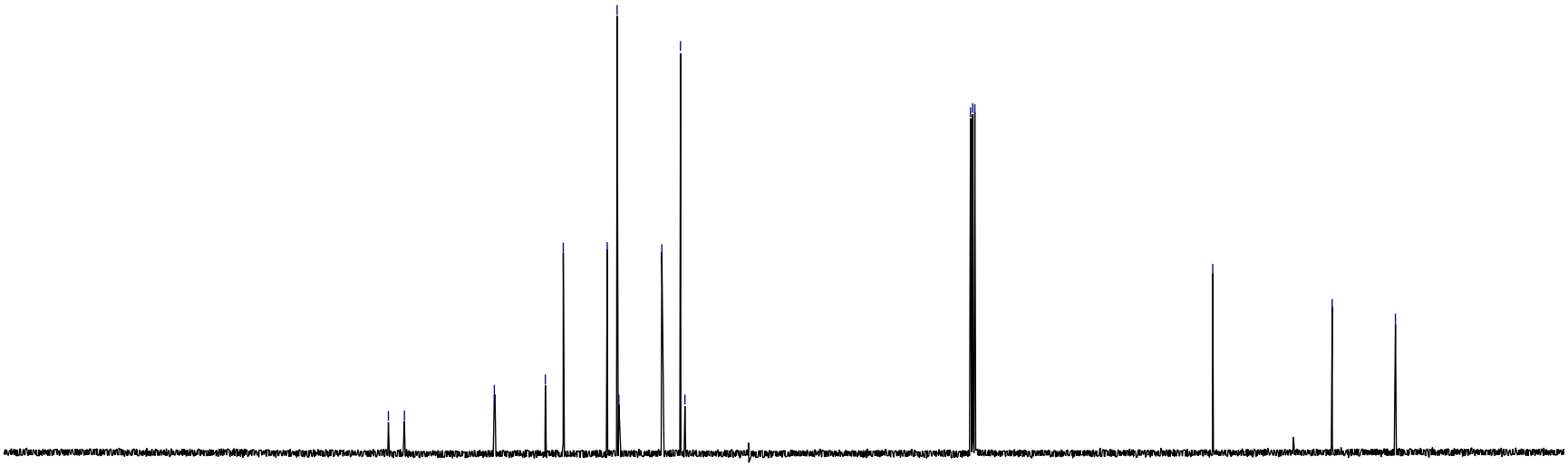


xg-3-69A-c13-

Parameter	Value
1 Title	xg-3-69A-c13-
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53
5 Nucleus	13C



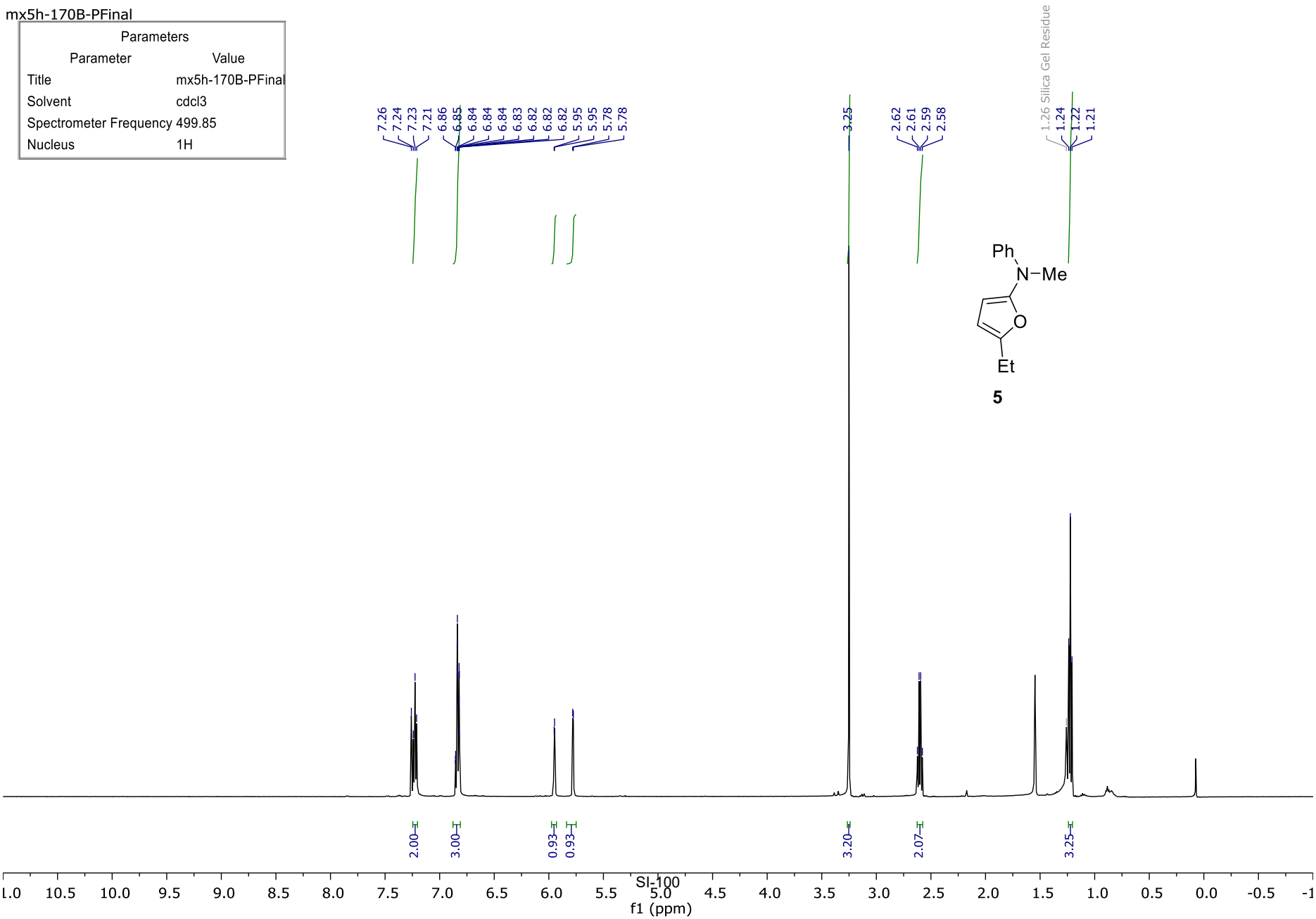
163.31
160.95
147.70
147.57
140.17
137.53
131.05
129.59
129.34
123.00
120.24
119.59
77.48
77.16
76.84
41.76
24.15
14.82



f1 (ppm)

mx5h-170B-PFinal

Parameters	
Parameter	Value
Title	mx5h-170B-PFinal
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H

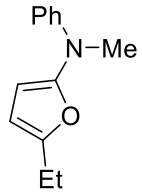


mx5c-170B-PFinal

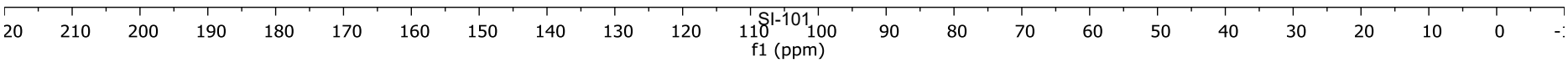
Std carbon

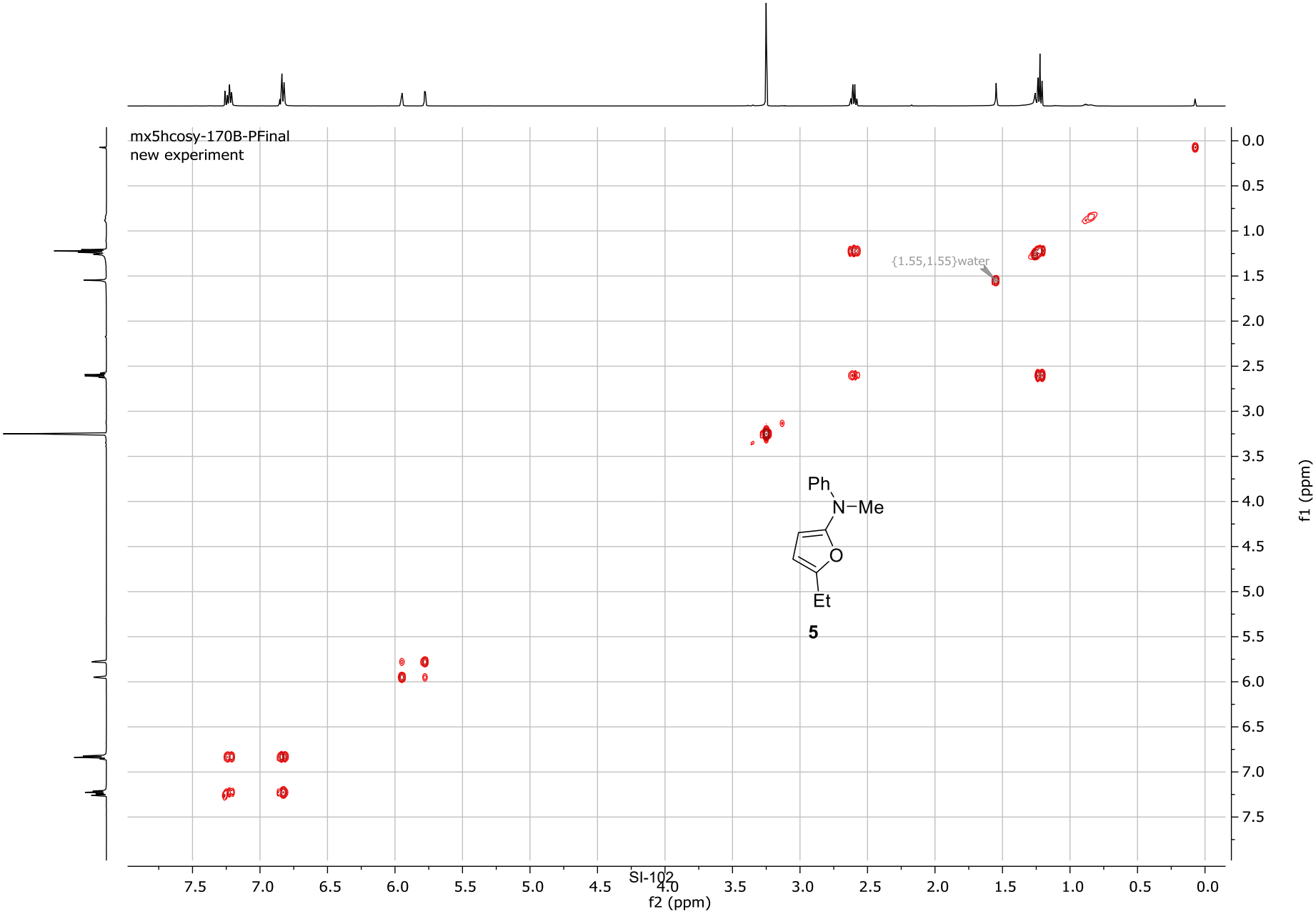
Parameters	
Parameter	Value
Title	mx5c-170B-PFinal
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

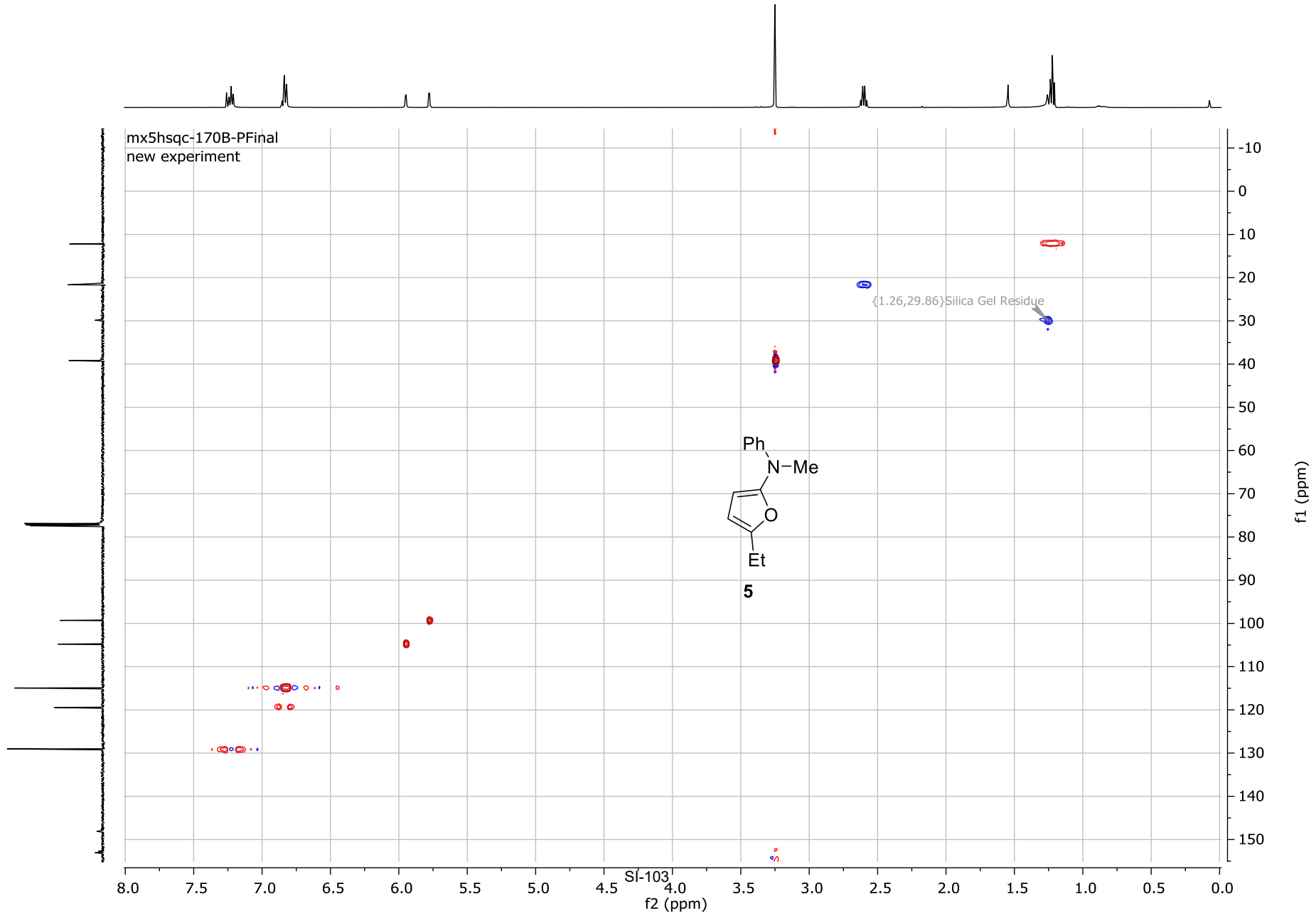
153.00
152.67
148.11
129.04
119.44
114.95
104.78
99.32
39.17
29.86 Silica Gel Residue
21.65
12.24

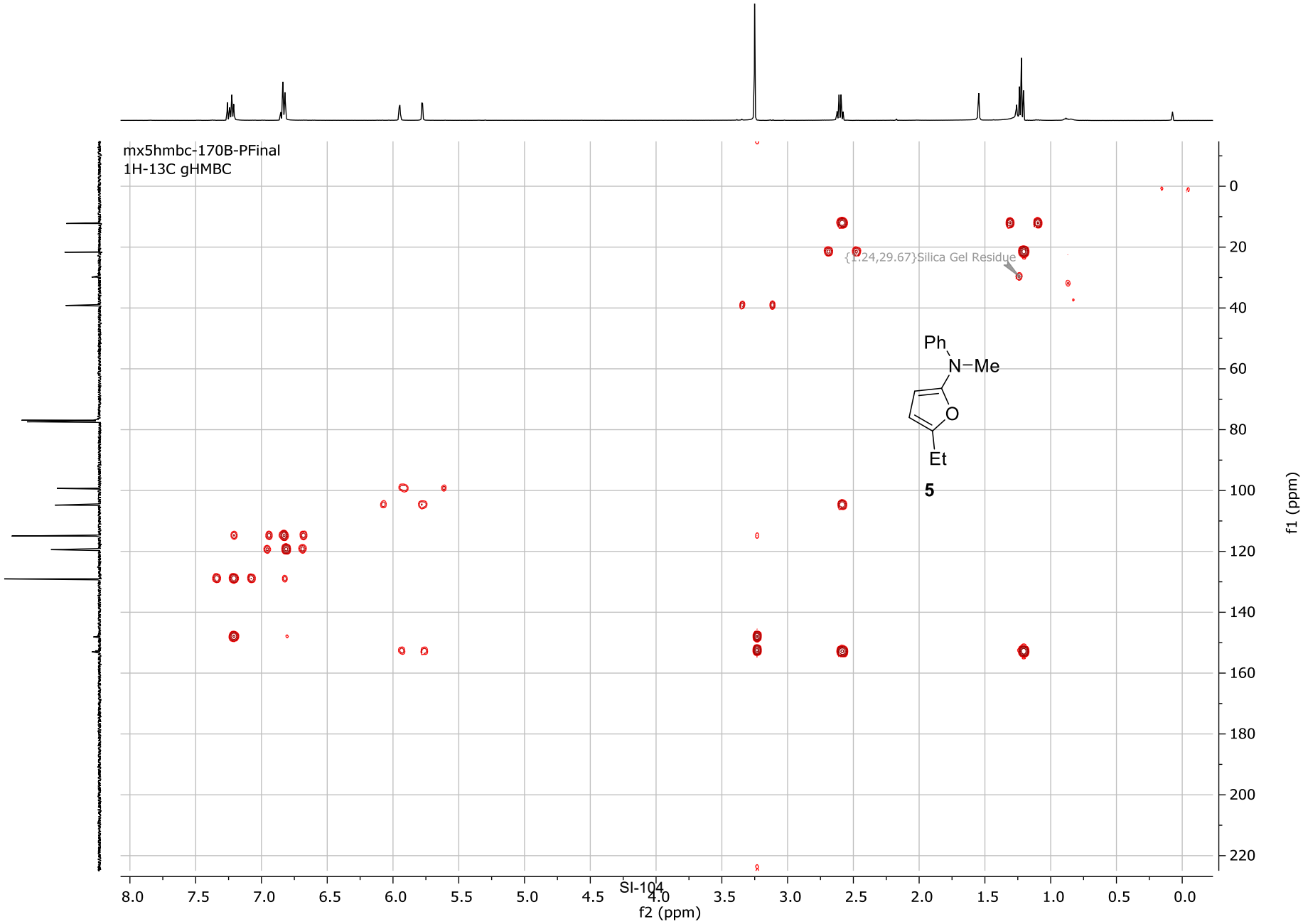


5




mx5hcosy-170B-PFinal
new experiment
{1.55,1.55}water
Ph
N−Me
O
Et
5
f2 (ppm)
f1 (ppm)

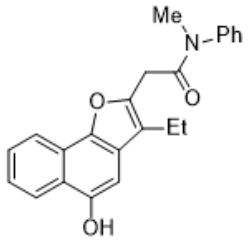

mx5hsqc-170B-PFinal
new experiment
{1.26,29.86}Silica Gel Residue
Ph
N−Me
O
Et
5
SI-103
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150


mx5hmbc-170B-PFinal
1H-13C gHMBC
{1.24,29.67}Silica Gel Residue
Ph
N–Me
O
Et
5
f2 (ppm)
f1 (ppm)
SI-104

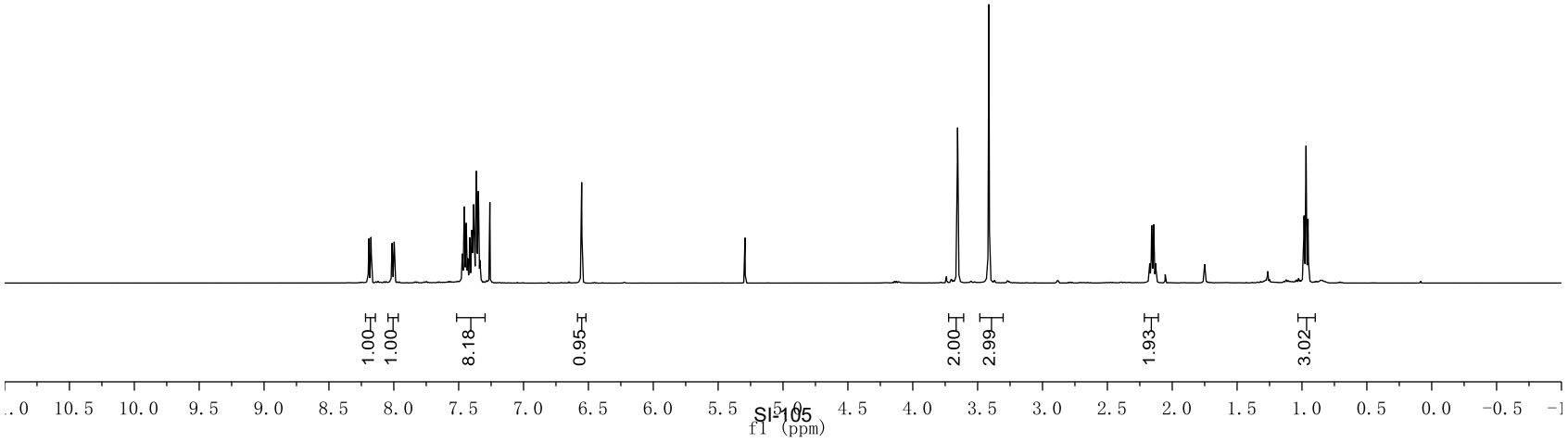
mx4h-195A-P

Parameters	
Parameter	Value
Title	mx4h-195A-P
Author	vnmr1
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H

8.09 8.08 8.01 8.00 7.47 7.46 7.44 7.42 7.41 7.40 7.39 7.39 7.38 7.37 7.36 7.36 7.36 7.35 7.35 7.35 7.35 7.26 6.55 — 5.29 DCM — 3.65 — 3.41 2.16 2.14 0.98 0.97 0.95

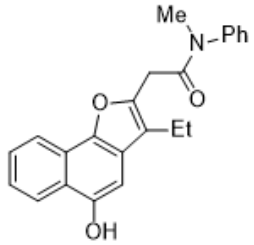


6

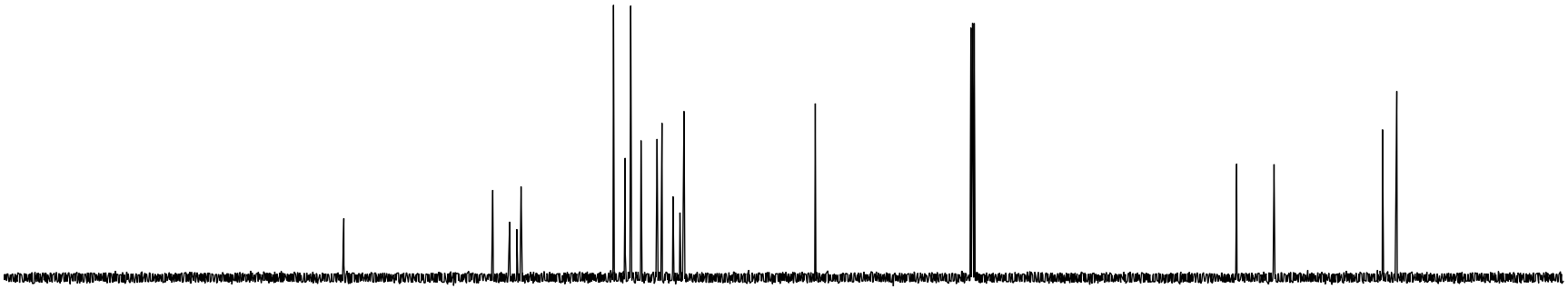


mx4c-195A-Ps5

169.87
147.91
145.41
144.36
143.74
130.11
128.38
127.56
126.05
123.78
123.68
123.08
122.96
121.33
120.30
119.71
77.41
77.16
76.91
38.22
32.70
16.70
14.60



6



f1 (ppm)

xg-2-243B-h

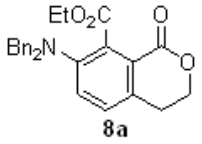
Parameters	
Parameter	Value
Title	xg-2-243B-h
Author	vnmr1
Solvent	CDCl3
Spectrometer Frequency	499.86
Nucleus	1H

7.31 7.30 7.29 7.29 7.27 7.26 7.25 7.22 7.22 7.22 7.21 7.21 7.20 7.19 7.16 7.15 7.11 7.09

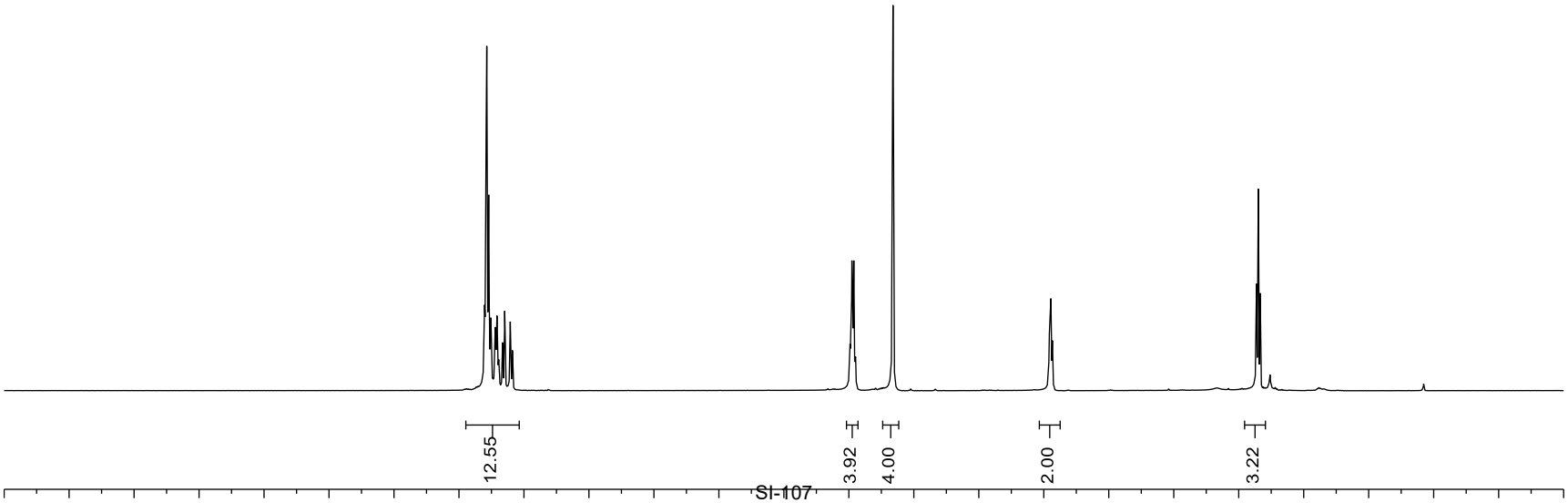
4.49 4.48 4.48 4.47 4.46 4.45 4.16

2.96 2.95 2.93

1.36 1.35 1.33



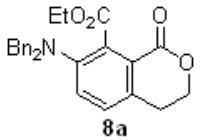
8a



xg-2-243B-c13

Parameters	
Parameter	Value
Title	xg-2-243B-c13
Author	
Solvent	CDCl3
Spectrometer Frequency	125.70
Nucleus	13C

168.40, 163.31, 148.43, 137.68, 135.50, 135.08, 129.14, 128.75, 128.35, 128.25, 127.23, 123.45, 77.41, 77.16, 76.91, 67.10, 61.99, 57.96, 27.79, 14.01



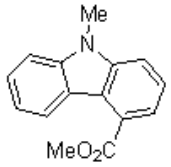
8a

f1 (ppm)

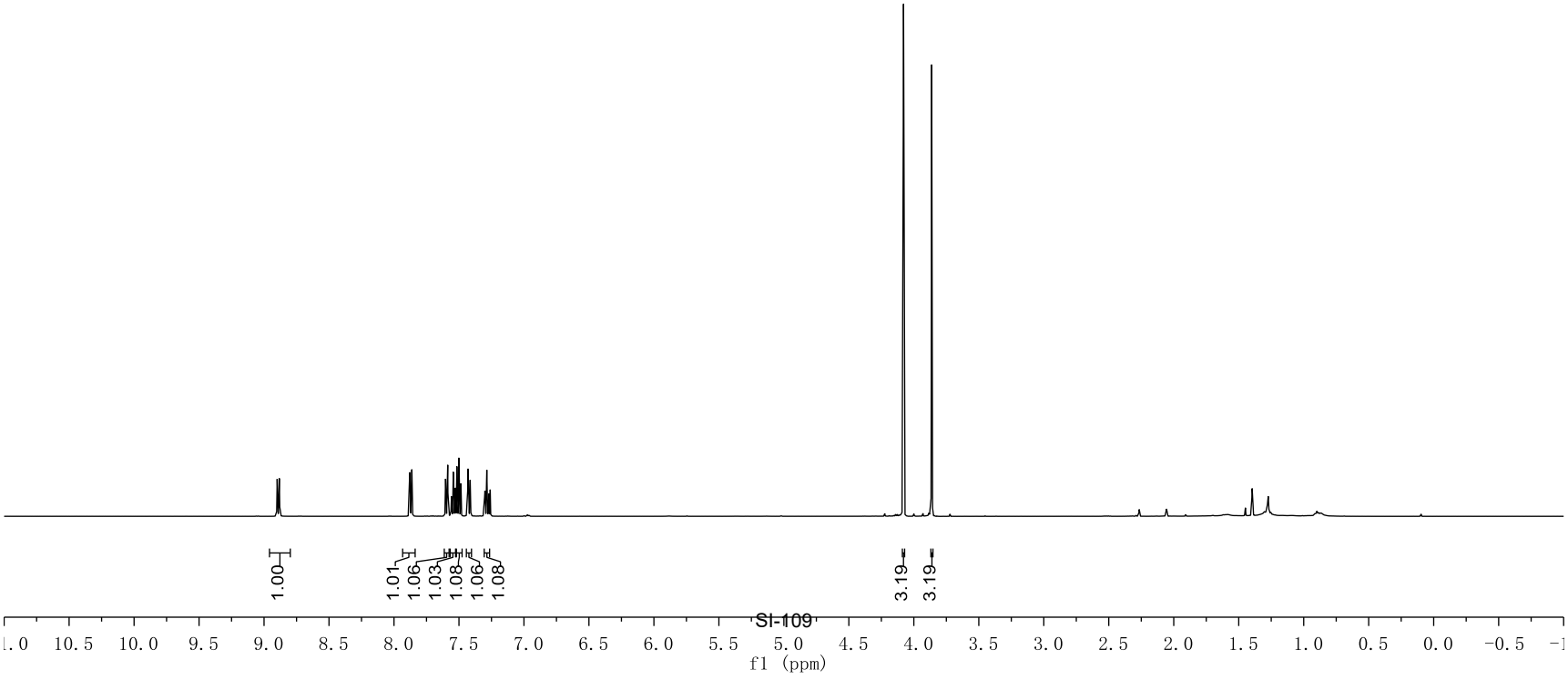
mx4h-189-8bPurified

Parameter	Value
Title	mx4h-189-8bPurified
Author	vnmr1
Solvent	cdcl3
Spectrometer Frequency	499.85
Nucleus	1H

8.90 8.90 8.90 8.88 8.88 8.88 7.88 7.88 7.86 7.86 7.60 7.60 7.59 7.59 7.54 7.54 7.53 7.53 7.52 7.50 7.50 7.48 7.43 7.43 7.43 7.41 7.41 7.30 7.30 7.29 7.29 7.28 7.27 7.27 7.26 4.08 3.86



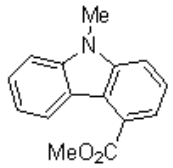
8b



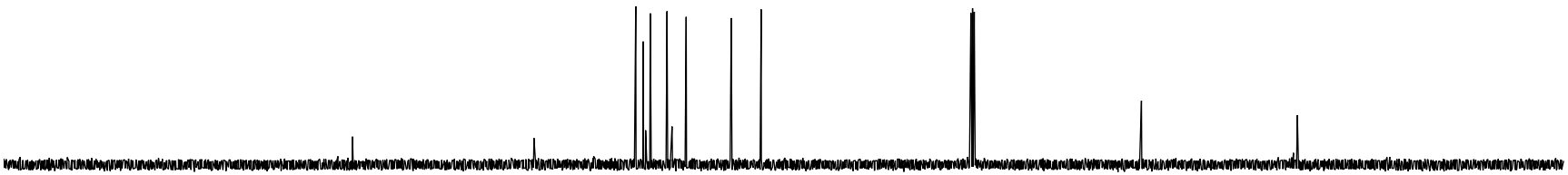
mx4c-189-8b-again

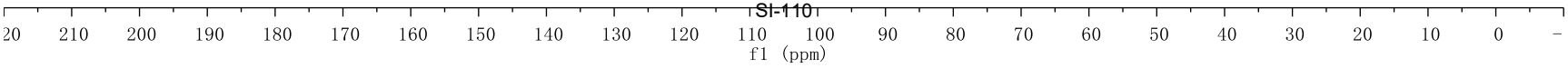
Parameters	
Parameter	Value
Title	mx4c-189-8b-again
Author	
Solvent	cdcl3
Spectrometer Frequency	125.70
Nucleus	13C

168.59
141.84
141.78
126.83
125.74
125.37
124.68
122.21
121.48
121.48
119.39
112.74
108.33
77.41
77.16
76.91
52.26
29.27



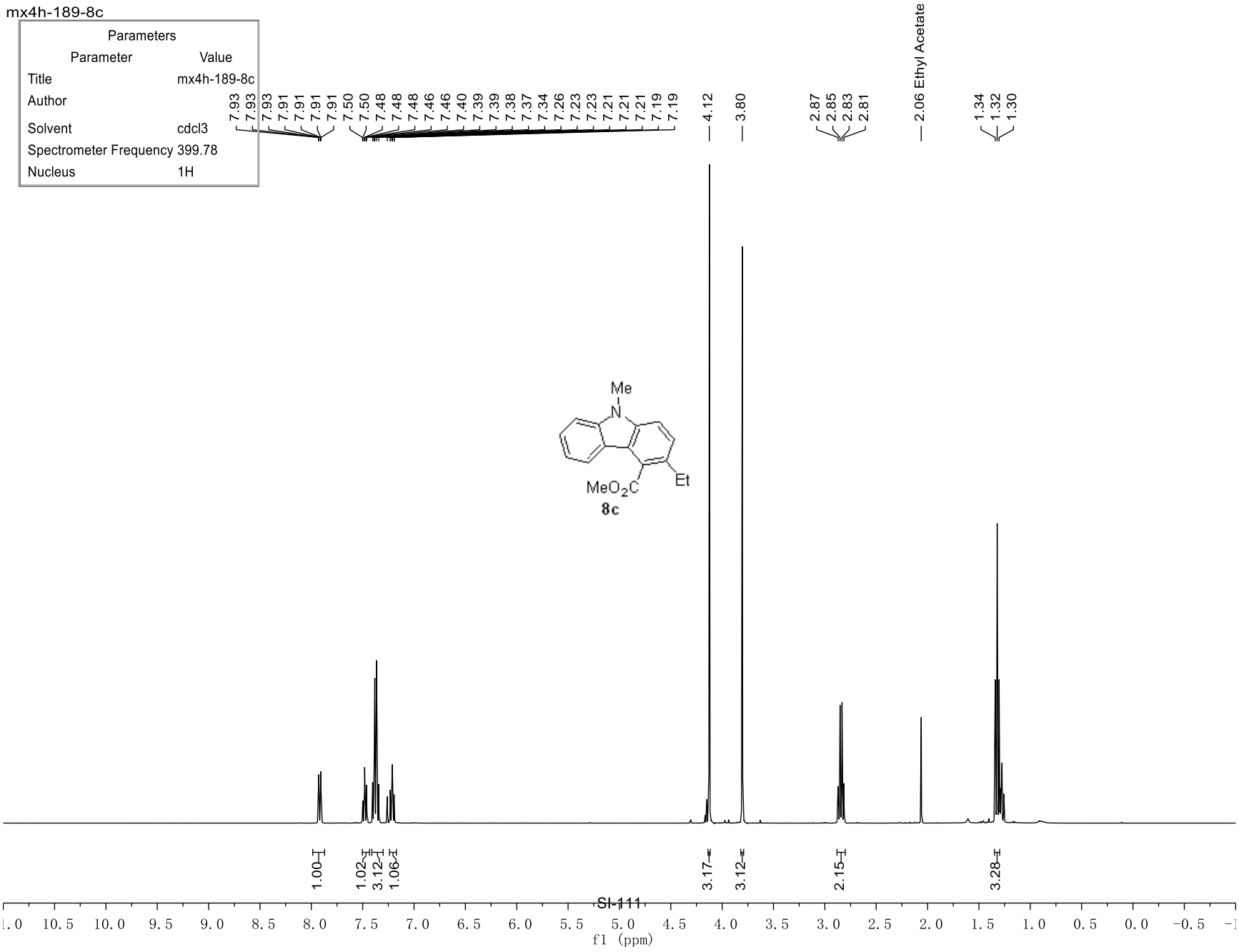
8b





mx4h-189-8c

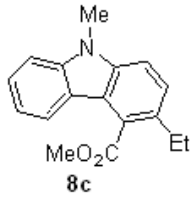
Parameters	
Parameter	Value
Title	mx4h-189-8c
Author	
Solvent	cdcl3
Spectrometer Frequency	399.78
Nucleus	1H



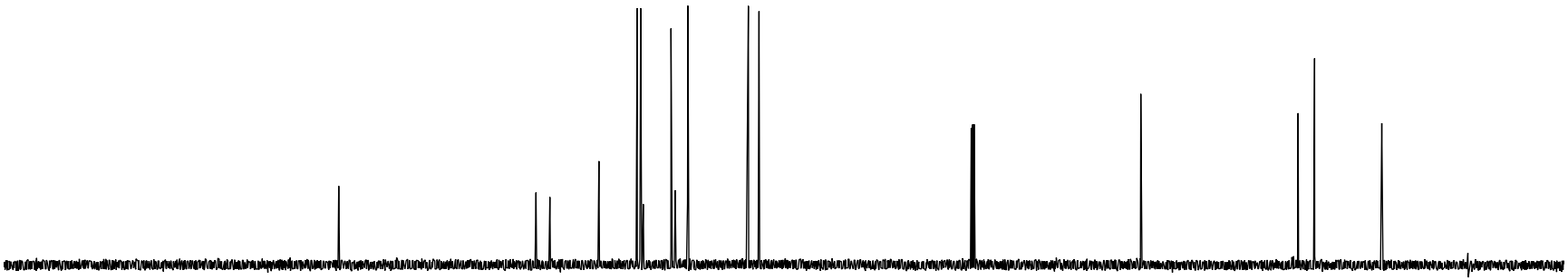
mx4c-189-8c

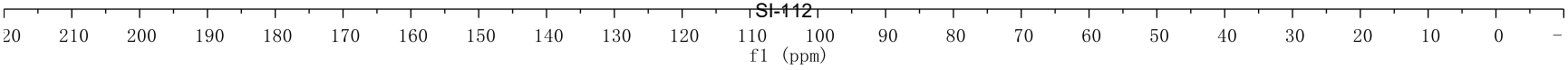
Parameters	
Parameter	Value
Title	mx4c-189-8c
Author	admin
Solvent	cdcl3
Spectrometer Frequency	150.79
Nucleus	13C

170.64
141.55
139.51
132.27
126.63
126.12
125.73
121.64
121.03
119.21
119.15
110.24
108.66
52.37
29.18
26.75
16.84



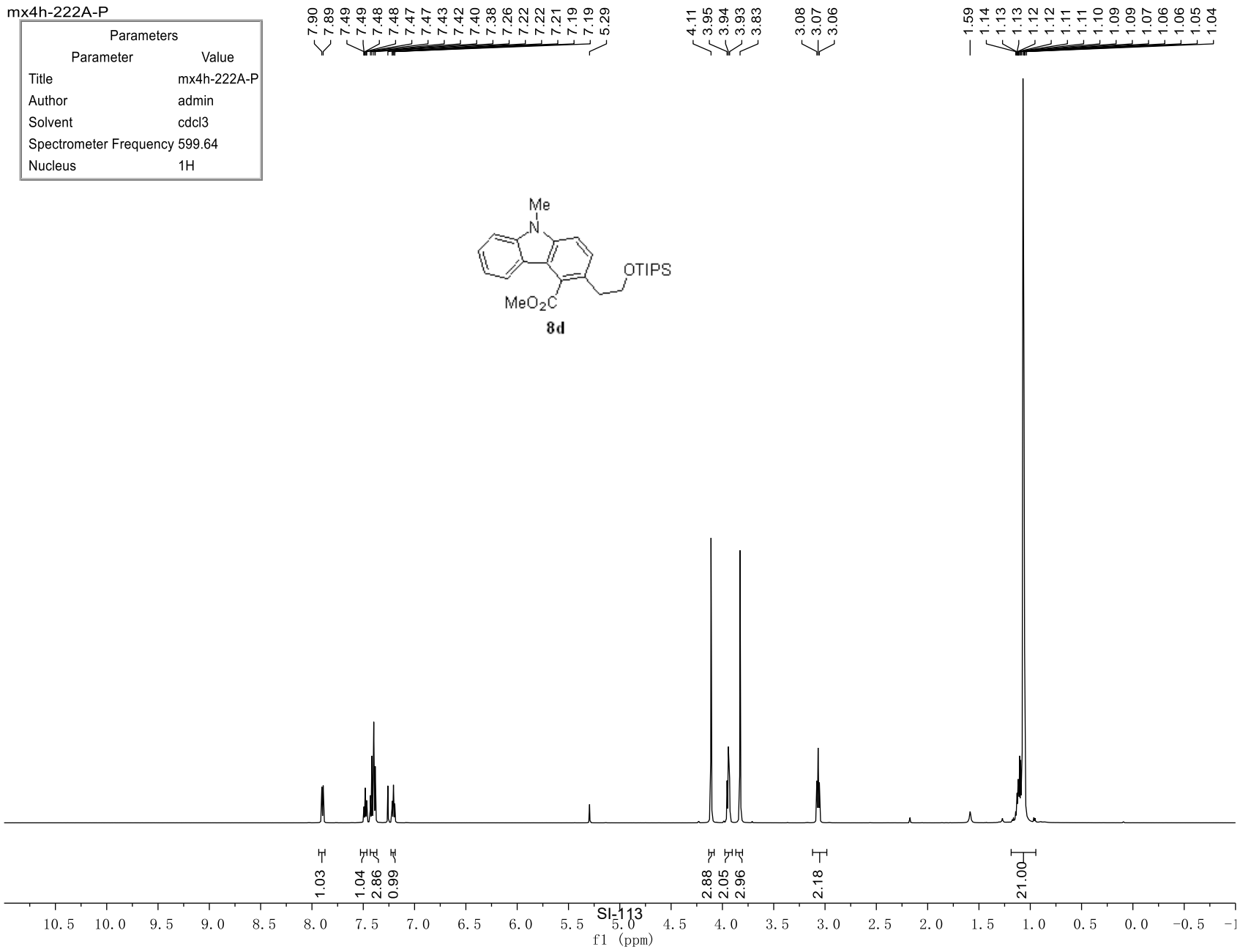
8c





mx4h-222A-P

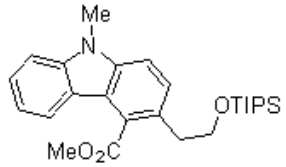
Parameters	
Parameter	Value
Title	mx4h-222A-P
Author	admin
Solvent	cdcl3
Spectrometer Frequency	599.64
Nucleus	1H



mx4c-222A-P

Parameters	
Parameter	Value
Title	mx4c-222A-P
Author	admin
Solvent	cdcl3
Spectrometer Frequency	150.79
Nucleus	13C

170.44
141.52
139.82
128.30
126.84
126.57
126.18
121.66
121.04
119.28
119.24
109.96
108.70
65.24
52.46
37.40
29.23
18.16
12.13



8d